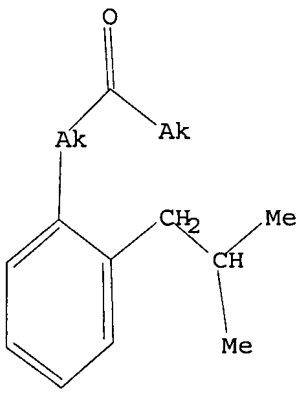
```
=> d his

     (FILE 'HOME' ENTERED AT 15:30:28 ON 03 NOV 2007)

     FILE 'REGISTRY' ENTERED AT 15:30:33 ON 03 NOV 2007
L1                SCREEN 1838 AND 1087
L2                STRUCTURE UPLOADED
L3                STRUCTURE UPLOADED
L4                STRUCTURE UPLOADED
L5                STRUCTURE UPLOADED
L6              0 S (L1 AND L2) SAM
L7              0 S (L1 AND L3) SAM
L8              0 S (L1 AND L4) SAM
L9              3 S (L1 AND L5) SAM
L10             0 S (L1 AND L2) SSS FULL
L11             1 S (L1 AND L3) SSS FULL
L12             7 S (L1 AND L4) SSS FULL
L13           183 S (L1 AND L5) SSS FULL
L14           190 S L10 OR L11 OR L12 OR L13

     FILE 'CAPLUS' ENTERED AT 15:33:08 ON 03 NOV 2007
L15           296 S L14

     FILE 'REGISTRY' ENTERED AT 15:33:15 ON 03 NOV 2007
                SAV TEM L14 ELE537824/A

     FILE 'STNGUIDE' ENTERED AT 15:34:54 ON 03 NOV 2007

     FILE 'REGISTRY' ENTERED AT 15:36:08 ON 03 NOV 2007
L16               STRUCTURE UPLOADED
L17             5 S L16 SAM SUB=L14
L18            85 S L16 SSS FULL SUB=L14

     FILE 'CAPLUS' ENTERED AT 15:36:49 ON 03 NOV 2007
L19           208 S L18
L20             1 S US200!-537824/APPS
L21           207 S L19 NOT L20

     FILE 'REGISTRY' ENTERED AT 15:37:26 ON 03 NOV 2007
                SAV TEM L18 NAR537824/A

     FILE 'CAPLUS' ENTERED AT 15:38:30 ON 03 NOV 2007

     FILE 'REGISTRY' ENTERED AT 15:38:52 ON 03 NOV 2007

     FILE 'STNGUIDE' ENTERED AT 15:39:34 ON 03 NOV 2007

     FILE 'CAPLUS' ENTERED AT 15:39:51 ON 03 NOV 2007

     FILE 'STNGUIDE' ENTERED AT 15:40:01 ON 03 NOV 2007

     FILE 'REGISTRY' ENTERED AT 15:42:21 ON 03 NOV 2007
L22               STRUCTURE UPLOADED
L23               STRUCTURE UPLOADED
L24             0 S L22 SAM SUB=L14
L25            19 S L22 SSS FULL SUB=L14
L26             0 S L23 SAM SUB=L14
L27            13 S L23 SSS FULL SUB=L14
L28            32 S L25 OR L27

     FILE 'CAPLUS' ENTERED AT 15:43:37 ON 03 NOV 2007
L29           163 S L28
L30           162 S L29 NOT L20
```

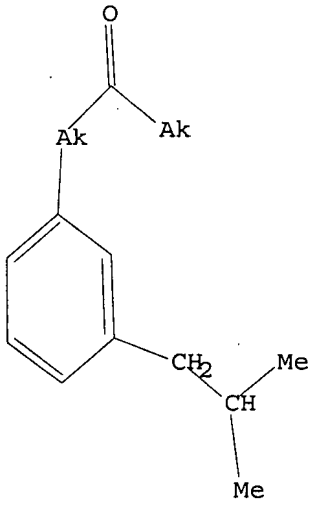
FILE 'REGISTRY' ENTERED AT 15:44:03 ON 03 NOV 2007

=> d l2
L2 HAS NO ANSWERS
L2 STR



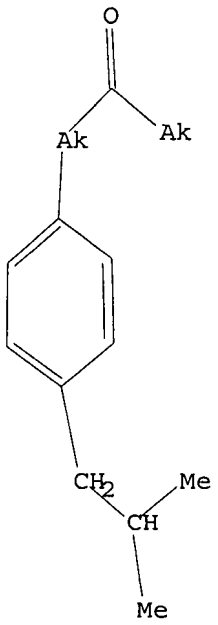

Structure attributes must be viewed using STN Express query preparation.

=> d l3
L3 HAS NO ANSWERS
L3 STR



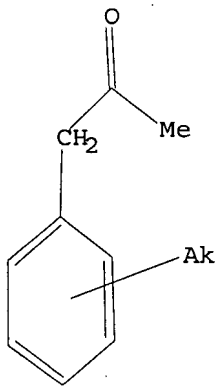

Structure attributes must be viewed using STN Express query preparation.

=> d l4
L4 HAS NO ANSWERS
L4 STR




Structure attributes must be viewed using STN Express query preparation.

=> d l5
L5 HAS NO ANSWERS
L5 STR




Structure attributes must be viewed using STN Express query preparation.

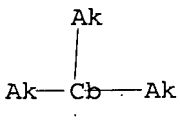
=> d l22
L22 HAS NO ANSWERS
L22 STR

Cb

Structure attributes must be viewed using STN Express query preparation.

=> d l23
L23 HAS NO ANSWERS

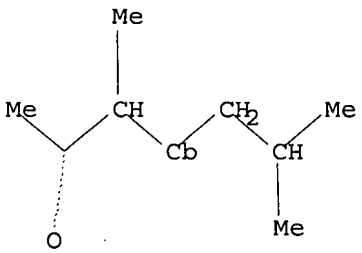
L23 STR




Structure attributes must be viewed using STN Express query preparation.

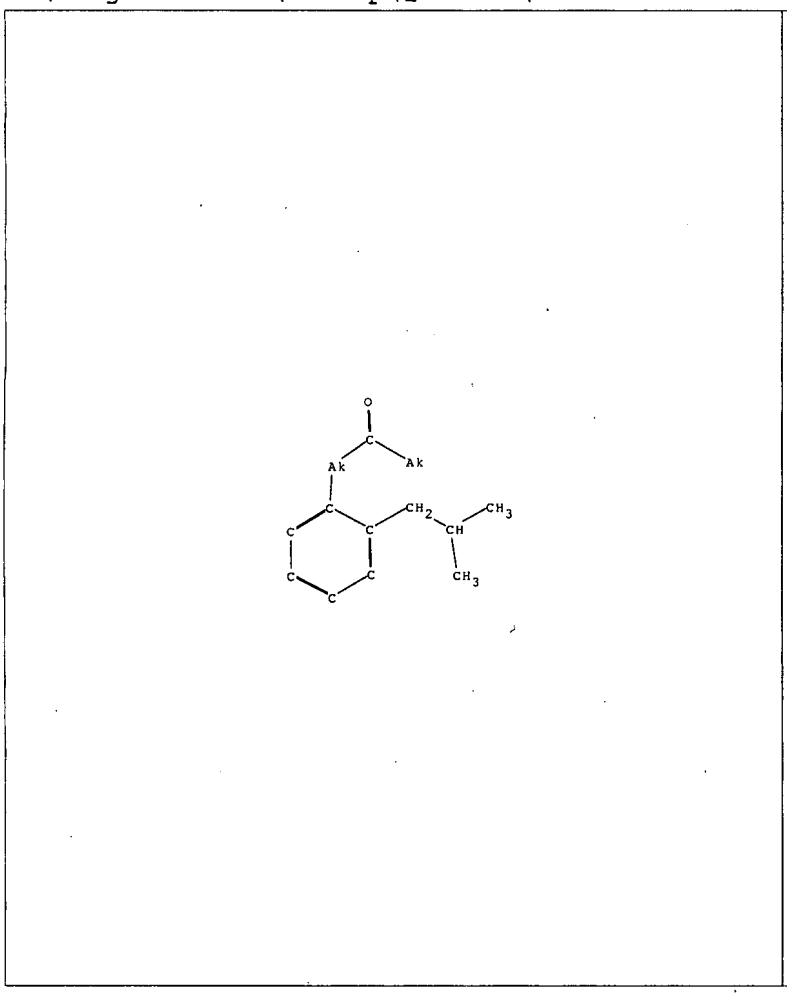
```
     FILE 'CAPLUS' ENTERED AT 15:43:37 ON 03 NOV 2007
L29           163 S L28
L30           162 S L29 NOT L20

     FILE 'REGISTRY' ENTERED AT 15:44:03 ON 03 NOV 2007

     FILE 'STNGUIDE' ENTERED AT 15:45:00 ON 03 NOV 2007

     FILE 'CAPLUS' ENTERED AT 15:46:14 ON 03 NOV 2007

=> s l30 and (method or pharma? or composition or treatment or medicament or
disease)
       3542142 METHOD
       1416321 METHODS
       4559136 METHOD
                 (METHOD OR METHODS)
        628669 PHARMA?
        706365 COMPOSITION
        323247 COMPOSITIONS
       1022238 COMPOSITION
                 (COMPOSITION OR COMPOSITIONS)
       1497406 COMPN
        603867 COMPNS
       1833701 COMPN
                 (COMPN OR COMPNS)
       2307904 COMPOSITION
                 (COMPOSITION OR COMPN)
       2350482 TREATMENT
        219539 TREATMENTS
       2466331 TREATMENT
                 (TREATMENT OR TREATMENTS)
          5888 MEDICAMENT
          5233 MEDICAMENTS
         10381 MEDICAMENT
                 (MEDICAMENT OR MEDICAMENTS)
       1003889 DISEASE
        272598 DISEASES
       1125534 DISEASE
                 (DISEASE OR DISEASES)
L31           60 L30 AND (METHOD OR PHARMA? OR COMPOSITION OR TREATMENT OR MEDICA
                 MENT OR DISEASE)
```

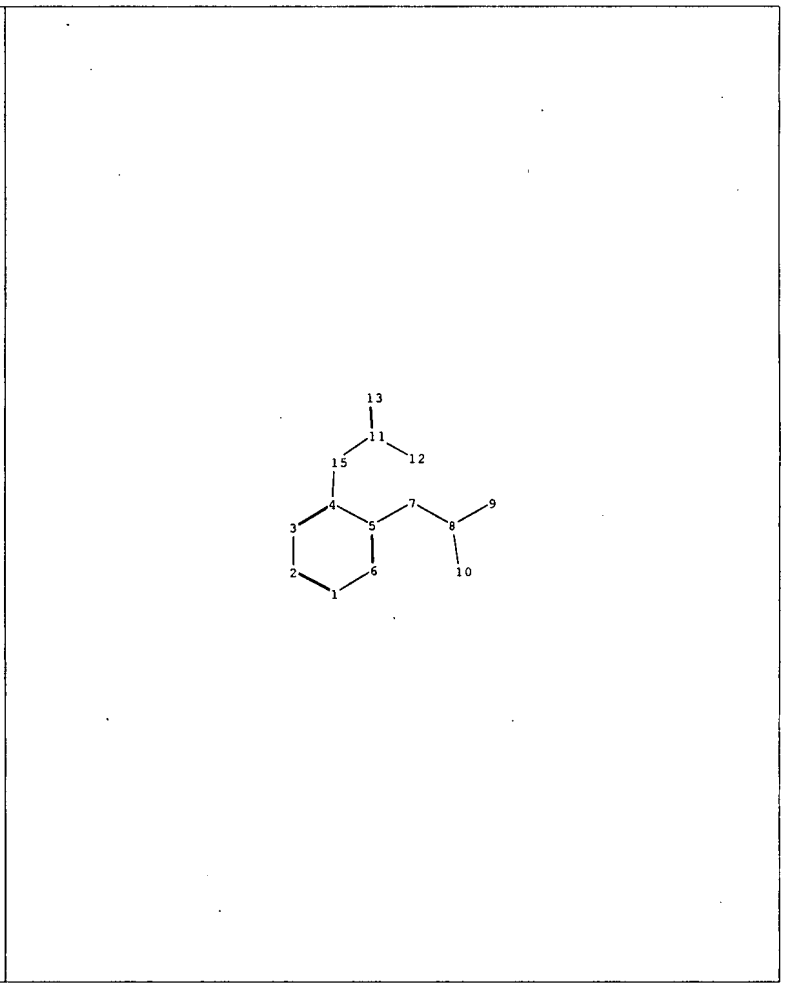
```
     FILE 'REGISTRY' ENTERED AT 15:53:09 ON 03 NOV 2007
L32             STRUCTURE UPLOADED
L33           0 S L32
L34             SCREEN 1838 AND 1087
L35             SCREEN 1838
L36           0 S (L35 AND L32) SAM
L37           2 S (L35 AND L32) SSS FULL
L38           0 S (L34 AND L32) SAM
L39           3 S (L34 AND L32) SSS FULL

     FILE 'CAPLUS' ENTERED AT 15:55:27 ON 03 NOV 2007
L40           5 S L39
L41           1 S US200!-537824/APPS
L42           4 S L40 NOT L41

     FILE 'REGISTRY' ENTERED AT 15:55:51 ON 03 NOV 2007

=> d l32
L32 HAS NO ANSWERS
L32             STR
```




Structure attributes must be viewed using STN Express query preparation.

C:\Program Files\Stnexp\Queries\10537824-F-1.str



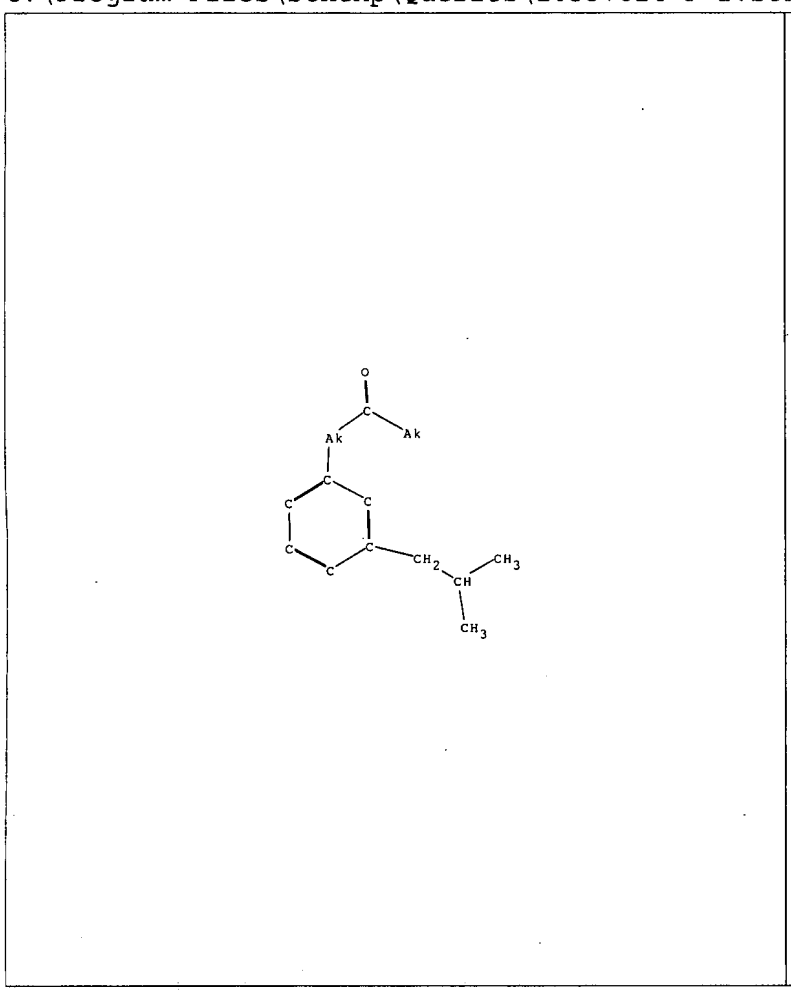



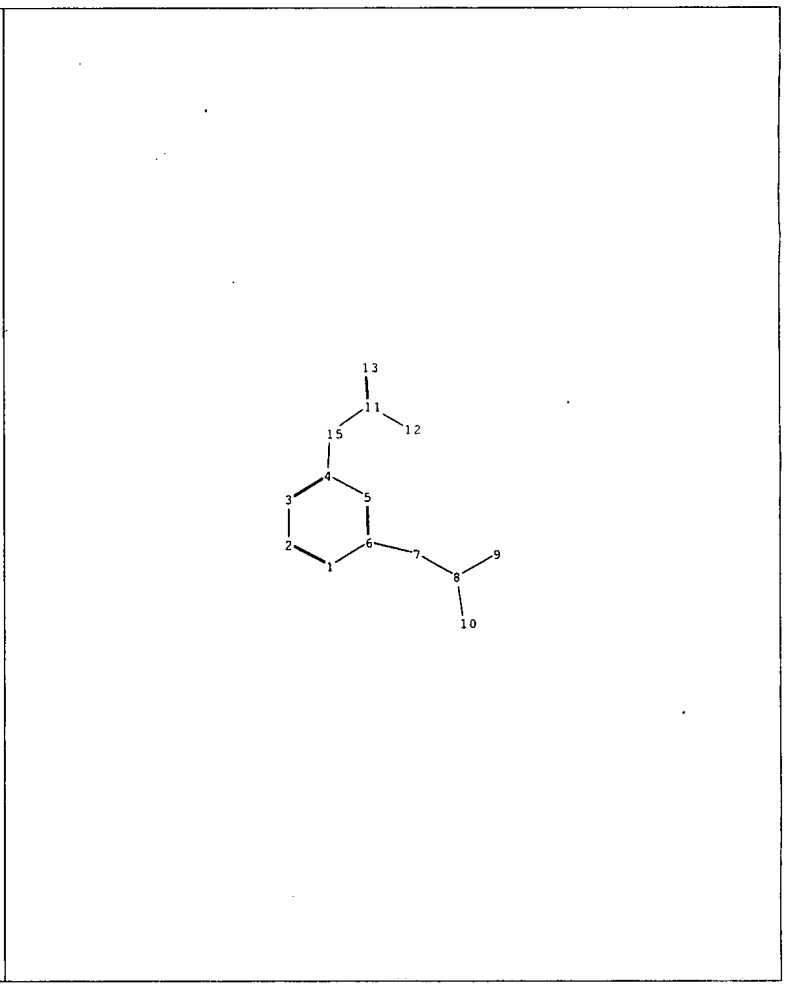

chain nodes :
7 8 9 10 11 12 13 15
ring nodes :
1 2 3 4 5 6
chain bonds :
4-15 5-7 7-8 8-9 8-10 11-13 11-12 11-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 11-13 11-12 11-15
exact bonds :
5-7 7-8 8-9 8-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Connectivity :
12:1 E exact RC ring/chain 15:2 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 15:CLASS
Generic attributes :
12:
Saturation : Saturated
15:

Saturation : Saturated

C:\Program Files\Stnexp\Queries\10537824-F-2.str



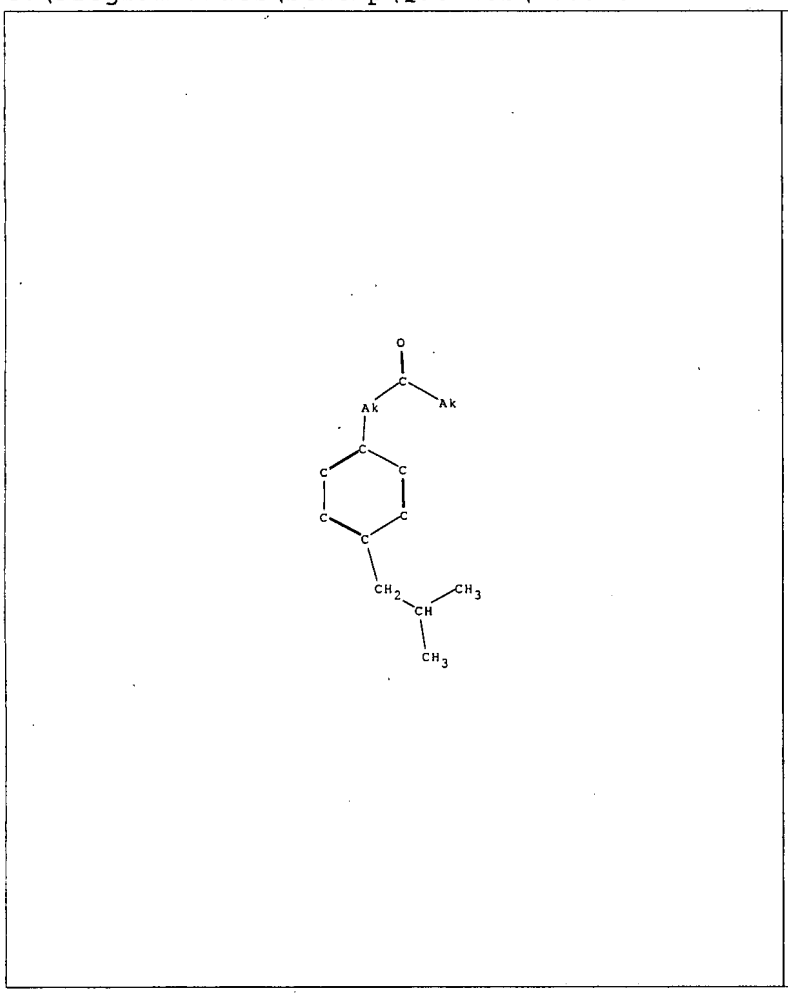



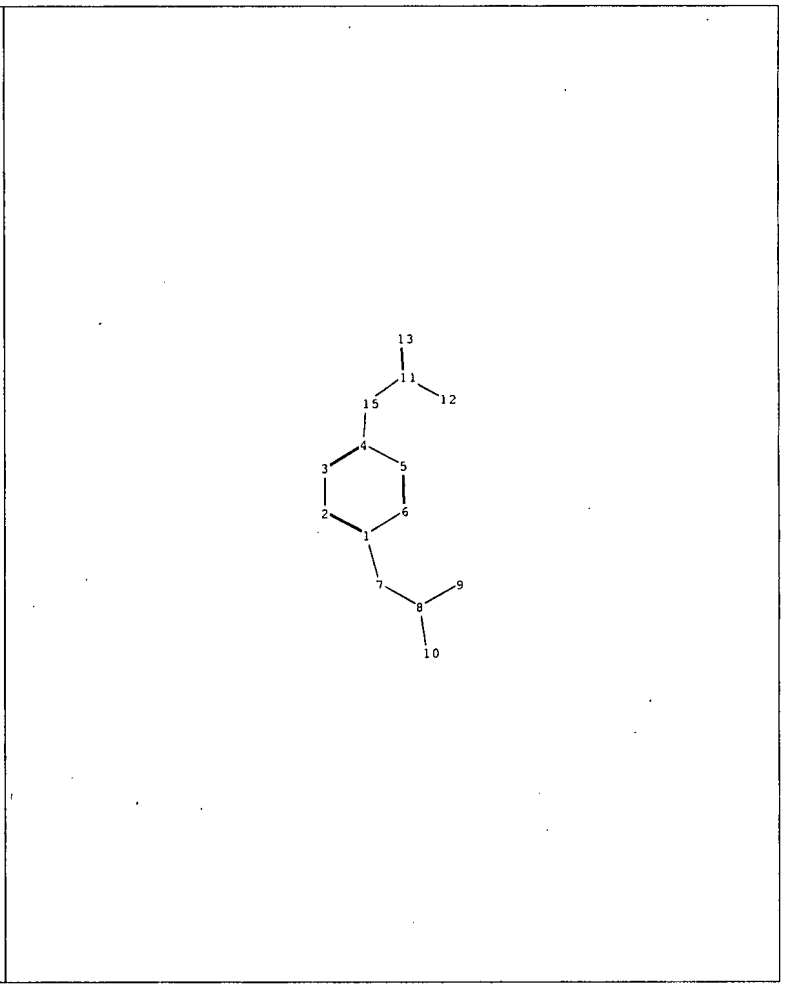

chain nodes :
7 8 9 10 11 12 13 15
ring nodes :
1 2 3 4 5 6
chain bonds :
4-15 6-7 7-8 8-9 8-10 11-13 11-12 11-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 11-13 11-12 11-15
exact bonds :
6-7 7-8 8-9 8-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Connectivity :
12:1 E exact RC ring/chain 15:2 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 15:CLASS
Generic attributes :
12:
Saturation : Saturated
15:

Saturation : Saturated

C:\Program Files\Stnexp\Queries\10537824-F-3.str



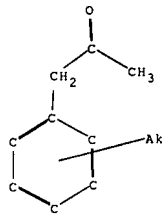



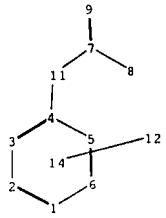

chain nodes :
7 8 9 10 11 12 13 15
ring nodes :
1 2 3 4 5 6
chain bonds :
1-7 4-15 7-8 8-9 8-10 11-13 11-12 11-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 11-13 11-12 11-15
exact bonds :
1-7 7-8 8-9 8-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Connectivity :
12:1 E exact RC ring/chain 15:2 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 15:CLASS
Generic attributes :
12:
Saturation : Saturated
15:

Saturation : Saturated

C:\Program Files\Stnexp\Queries\10537824-F-4.str

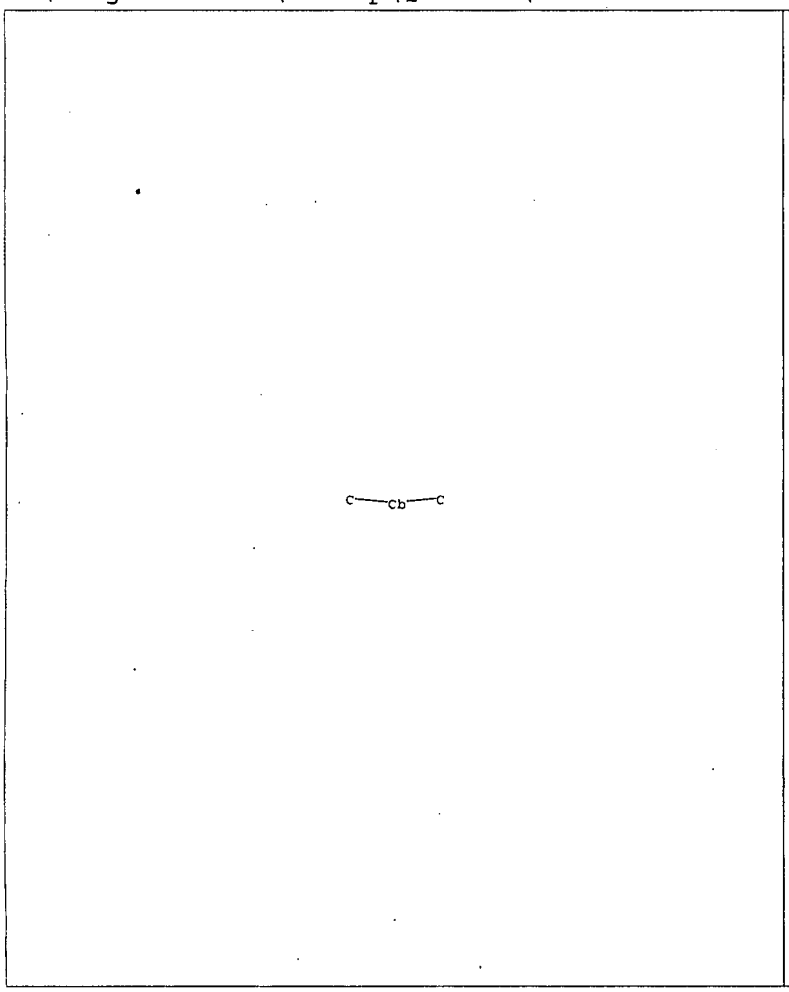


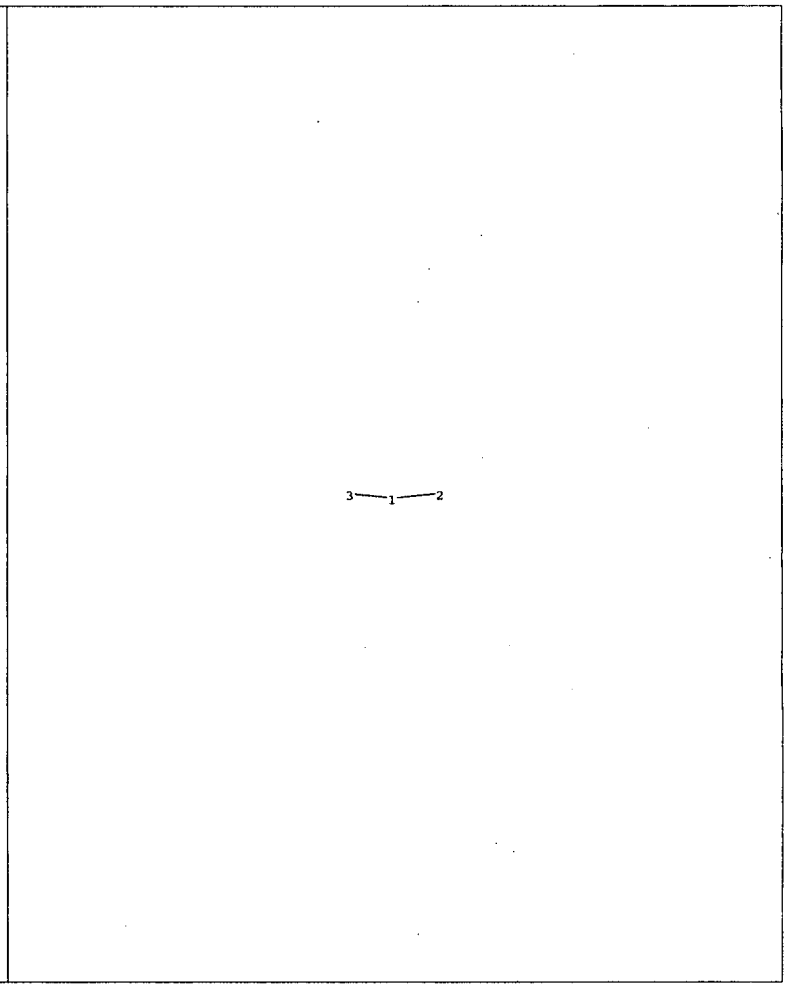




chain nodes :
7 8 9 11 12
ring nodes :
1 2 3 4 5 6
chain bonds :
4-11 7-9 7-8 7-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
7-9
exact bonds :
4-11 7-8 7-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Connectivity :
12:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 14:Atom
Generic attributes :
12:
Saturation : Saturated

C:\Program Files\Stnexp\Queries\10537824-narrow-F1.str



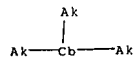



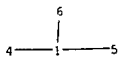

chain nodes :
    1  2  3
chain bonds :
    1-2  1-3
exact bonds :
    1-2  1-3

Connectivity :
    1:2 E exact RC ring/chain
Match level :
    1:Atom  2:CLASS  3:CLASS
Generic attributes :
    1:
    Saturation              : Unsaturated
    Number of Carbon Atoms  : less than 7
    Type of Ring System     : Monocyclic

Element Count :
    Node 1: Limited
        C,C6

C:\Program Files\Stnexp\Queries\10537824-narrow-F2.str



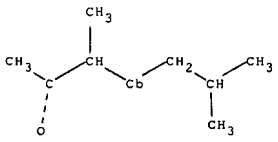



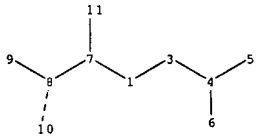

chain nodes :
    1  4  5  6
chain bonds :
    1-4  1-5  1-6
exact/norm bonds :
    1-4  1-5  1-6

Connectivity :
    1:3 E exact RC ring/chain  6:1 E exact RC ring/chain
Match level :
    1:Atom  4:CLASS  5:CLASS  6:CLASS
Generic attributes :
    1:
    Saturation              : Unsaturated
    Number of Carbon Atoms  : less than 7
    Type of Ring System     : Monocyclic
    6:
    Saturation              : Saturated

Element Count :
    Node 1: Limited
        C,C6

C:\Program Files\Stnexp\Queries\10537824-species.str




chain nodes :
1 3 4 5 6 7 8 9 10 11
chain bonds :
1-3 1-7 3-4 4-5 4-6 7-8 7-11 8-9 8-10
exact/norm bonds :
8-10
exact bonds :
1-3 1-7 3-4 4-5 4-6 7-8 7-11 8-9

Connectivity :
1:2 E exact RC ring/chain
Match level :
1:Atom 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS
Generic attributes :
1:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

L41 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:515465 CAPLUS
DN 141:54204
TI Preparation of chiral aryl ketones in the treatment of neutrophil-dependent inflammatory diseases
IN Allegretti, Marcello; Bertini, Riccardo; Cesta, Maria Candida; Bizzarri, Cinzia; Colotta, Francesco
PA Dompe S.P.A., Italy
SO PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

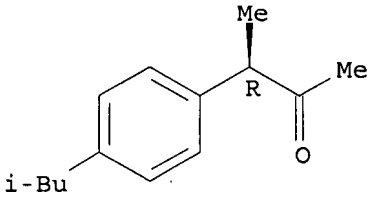
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2004052830 | A1 | 20040624 | WO 2003-EP13946 | 20031209 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| | RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2507765 | A1 | 20040624 | CA 2003-2507765 | 20031209 |
| | AU 2003289993 | A1 | 20040630 | AU 2003-289993 | 20031209 |
| | EP 1581474 | A1 | 20051005 | EP 2003-782344 | 20031209 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| | CN 1732145 | A | 20060208 | CN 2003-80107685 | 20031209 |
| | JP 2006509022 | T | 20060316 | JP 2004-558041 | 20031209 |
| | NO 2005003086 | A | 20050623 | NO 2005-3086 | 20050623 |
| | US 2006247297 | A1 | 20061102 | US 2006-537824 | 20060208 <-- |
| PRAI | EP 2002-27453 | A | 20021210 | | |
| | WO 2003-EP13946 | W | 20031209 | | |

OS MARPAT 141:54204
AB (R,S)-1-arylethyl ketone compds. of formula ArCH(Me)COCH(Ra)Rb and their single (R) and (S) enantiomers [wherein Ar = aryl; Ra, Rb = H, linear or branched C1-6 alkyl, Ph, α- or β-naphthyl, 2-, 3-, or 4-pyridyl, C1-4-alkylphenyl, C1-4 alkyl(α- or β-naphthyl), C1-4 alkyl(2-, 3-, or 4-pyridyl), cyano, carboxyamide, CO2H or its esters of formula CO2R" (wherein R" = the residue of linear or branched C1-6 aliphatic alc.), a phosphonate of formula PO(OR")2 (wherein R" is as defined above), a group of formula di-X-(CH2)n-Z (wherein X = CO, SO, SO2; Z = H, tert-Bu, iso-Pr, CO2R'', cyano, Ph, α- or β-naphthyl, 2-, 3-, or 4-pyridyl, C3-6 cycloalkyl, NH-BOC, NH2; n = 0 or an integer from 1 to 3; or Ra and Rb, with the carbon atom to which they are bound, form a cyclic residue 2,2-di(R')-substituted 4,6-dioxo-1,3-dioxane; wherein R' = Me or Et, or the two groups R' form a cyclohexane or cyclopentane ring)] are prepared These compds. are useful in therapy as drugs for the treatment of diseases mediated by infiltrations of neutrophils induced by IL-8, such as psoriasis, rheumatoid arthritis, ulcerative colitis, acute respiratory distress syndrome (ARDS), idiopathic fibrosis, glomerulonephritis, bollous pemphigo and for the prevention and the treatment of damages caused by ischemia and reperfusion. Thus, (R)-(-)-ibuprofen (2 g, 9.69 mmol) was dissolved in 4 mL SOCl2 and refluxed for 4 h to give, after evaporation, (R)-2-(4-Isobutylphenyl)propanoyl chloride as an oily yellow residue (2.34 g; 9.34 mmol). The oil was dissolved in dry 3 mL CH2Cl2 and the resulting solution was added to a solution of 2,2-dimethyl-1,3-dioxan-2,5-dione (Meldrum's acid) (1.35 g; 9.34 mmol) and pyridine (1.83 mL; 22.9 mmol) in dry CH2Cl2

(7.5 mL) previously cooled to 0-5° with a water/ice bath, and left for 1 h at this temperature and then for another hour at room temperature to give, after workup, 2.69 g (R)-(+)-5-[2-(4-isobutylphenyl)propion-1-yl]-2,2-dimethyl-1,3-dioxan-4,6-dione. The latter compound was dissolved in dioxane (10 mL), treated with glacial acetic acid (0.84 mL) and H2O (0.13 mL), and heated to the reflux temperature for 3 h to give, after cooling and evaporation of the solvents and purification by means of flash chromatog. (R)-(-)-3-(4-isobutylphenyl)butan-2-one as a pale yellow oil (0.97 g; 4.75 mmol).

L42 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:460353 CAPLUS
DN 143:145782
TI 2-Arylpropionic CXC Chemokine Receptor 1 (CXCR1) Ligands as Novel Noncompetitive CXCL8 Inhibitors
AU Allegretti, Marcello; Bertini, Riccardo; Cesta, Maria Candida; Bizzarri, Cinzia; Di Bitondo, Rosa; Di Cioccio, Vito; Galliera, Emanuela; Berdini, Valerio; Topai, Alessandra; Zampella, Giuseppe; Russo, Vincenzo; Di Bello, Nicoletta; Nano, Giuseppe; Nicolini, Luca; Locati, Massimo; Fantucci, Piercarlo; Florio, Saverio; Colotta, Francesco
CS Dompe Research and Development, Dompe S.p.A., L'Aquila, 67100, Italy
SO Journal of Medicinal Chemistry (2005), 48(13), 4312-4331
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 143:145782
AB The CXC chemokine CXCL8/IL-8 plays a major role in the activation and recruitment of polymorphonuclear (PMN) cells at inflammatory sites. CXCL8 activates PMNs by binding the seven-transmembrane (7-TM) G-protein-coupled receptors CXC chemokine receptor 1 (CXCR1) and CXC chemokine receptor 2 (CXCR2). (R)-Ketoprofen (1) was previously reported to be a potent and specific noncompetitive inhibitor of CXCL8-induced human PMNs chemotaxis. The authors report here mol. modeling studies showing a putative interaction site of 1 in the TM region of CXCR1. The binding model was confirmed by alanine scanning mutagenesis and photoaffinity labeling expts. The mol. model driven medicinal chemical optimization of 1 led to a new class of potent and specific inhibitors of CXCL8 biol. activity. Among these, repertaxin was selected as a clin. candidate drug for prevention of postischemia reperfusion injury.
IT 709039-97-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(2-arylpropionic CXC chemokine receptor 1 (CXCR1) ligands as novel noncompetitive CXCL8 inhibitors)
RN 709039-97-4 CAPLUS
CN 2-Butanone, 3-[4-(2-methylpropyl)phenyl]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).




RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1991:228497 CAPLUS
DN 114:228497
TI 2-(4-Isobutylphenyl)-2-butene as intermediate for ibuprofen
IN Shimizu, Isoo; Matsumura, Yasuo; Uchida, Kazumichi; Tokumoto, Yuichi
PA Nippon Petrochemicals Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DT Patent
LA Japanese

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | JP 03024023 | A | 19910201 | JP 1989-160325 | 19890622 |
| PRAI | JP 1989-160325 | | 19890622 | | |

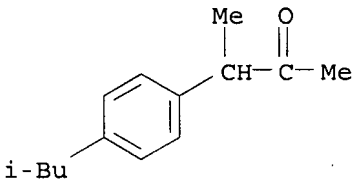
OS CASREACT 114:228497

AB The title compound (I), useful as intermediate for ibuprofen, was prepared Four portions of Me3COK were successively added to a mixture of Ph3EtP+ Br- and THF at room temperature over 30 min, 40.5 g 4-Me2CHCH2C6H4COMe was added dropwise over 1 h, then the reaction mixture was further stirred for 2 h to give 27 g I. A mixture of I, PhI(OAc)2, Co(OAc)2.4H2O, and AcOH was stirred at 25° for 4 h to give 87% 4-Me2CHCH2C6H4CHMeCOMe (II) at 99% conversion. An aqueous NaOCl solution was added dropwise to a MeOH solution of II at -10° over 1 h and the reaction mixture was further stirred for 5 h to give ibuprofen.

IT 64758-90-3P, 3-(4-Isobutylphenyl)-2-butanone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and haloform reaction of, ibuprofen from)

RN 64758-90-3 CAPLUS

CN 2-Butanone, 3-[4-(2-methylpropyl)phenyl]- (9CI) (CA INDEX NAME)




L42 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1978:169781 CAPLUS

DN 88:169781

TI 2-(4-Alkylphenyl)propionic acids

IN Yamada, Yoshitsugu

PA Mitsui Toatsu Chemicals, Inc., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

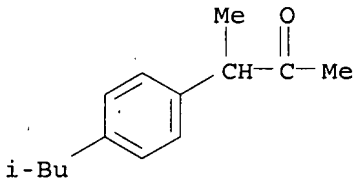
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | JP 52108949 | A | 19770912 | JP 1976-23080 | 19760305 |
| | JP 58042851 | B | 19830922 | | |
| PRAI | JP 1976-23080 | A | 19760305 | | |

AB RPh (R = alkyl) were treated with AcAc to give p-RC6H4CMe(OH)Ac (I), which were reduced to p-RC6H4CHMeAc (II) and oxidized to give p-RC6H4CHMeCO2H (III). III are analgesics and antiinflammatory agents (no data). Thus, 0.75 mol iso-BuPh was treated with AlCl3, and 0.058 mol AcAc to give 33.6% I (R = iso-Bu), which in PhCl was reduced by Zn-Hg and HCl 1 h at 65-70° to give 86.4% II (R = iso-Bu). This was oxidized by NaOH-Br2 in dioxane-H2O 2 h to give 91.7% III.

IT 64758-90-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation by bromine and sodium hydroxide)

RN 64758-90-3 CAPLUS

CN 2-Butanone, 3-[4-(2-methylpropyl)phenyl]- (9CI) (CA INDEX NAME)

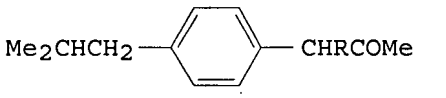



L42 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1977:601111 CAPLUS
DN 87:201111
TI 2-(4-Isobutylphenyl)propionic acid
IN Matsumura, Takumi; Tani, Katsuya
PA Daito Koeki Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | JP 52083426 | A | 19770712 | JP 1975-158427 | 19751230 |
| PRAI | JP 1975-158427 | A | 19751230 | | |

GI

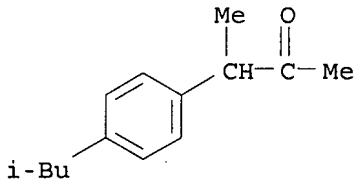



II, R=H
III, R=Me

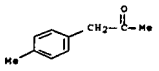
AB Antiinflammatory (no data) title acid (I) was prepared by methylating II to III, followed by oxidation with NaOBr. Thus, 29 g II was treated with MeI and NaH in C6H6 to give 20 g III, which was oxidized to I with NaOBr in aqueous dioxane.

IT 64758-90-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

RN 64758-90-3 CAPLUS
CN 2-Butanone, 3-[4-(2-methylpropyl)phenyl]- (9CI) (CA INDEX NAME)



L31 ANSWER 1 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:769733 CAPLUS Full-text
DN 147:343757
TI Heck reactions of α- or β-substituted enol ethers with aryl bromides catalyzed by a tetraphosphane/palladium complex-direct access to acetophenone or 1-arylpropanone derivatives
AU Battace, Ahmed; Feuerstein, Marie; Lemhadri, Mhamed; Zair, Touriya; Doucet, Henri; Santelli, Maurice
CS Laboratoire de Synthese Organique associe au CNRS, Faculte des Sciences de Saint Jerome, Universite d'Aix-Marseille, Marseille, 13397, Fr.
SO European Journal of Organic Chemistry (2007), (19), 3122-3132
CODEN: EJOCFK; ISSN: 1434-193X
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
AB Cis,cis,cis-1, 2,3,4-Tetrakis(diphenylphosphanylmethyl)cyclopentane/[PdCl(C3H5)]2 efficiently catalyzes the Heck reaction of α- and β-substituted enol ethers with aryl bromides. The arylation of 1-phenyl-1-(trimethylsilyloxy)ethylene led directly to the 2-aryl-1-phenylethanones. Similar reaction rates were observed with electron-rich, electron-deficient or sterically congested aryl bromides. Heck reaction with benzyl isopropenyl ether gave a mixture of isomers. However, this mixture gave selectively the 1-arylpropanones after hydrolysis. Employing β-methoxystyrene, 3-ethoxyacrylonitrile or Me 3-methoxyacrylate, the regioselective α-arylation of these enol ethers was observed in all cases, but mixts. of (Z) and (E) isomers were generally obtained, which in many cases yielded a single ketone product after acid treatment. The stereoselectivity of this reaction depends on steric and electronic factors, and better stereoselectivities in favor of (Z) isomers were observed with electron-rich or sterically congested aryl bromides. Higher yields were obtained for this reaction with electron-rich or sterically congested aryl bromides than with electron-poor aryl bromides. These observations suggest that the rate-limiting step of the catalytic cycle is not the oxidative addition of the aryl bromide to the palladium complex with these substituted enol ethers.
IT 2096-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of arylketones via palladium-tedicyp-catalyzed Heck reaction of haloarenes with (silyloxy)ethenylbenzene, benzyloxypropene, methoxystyrene or (methoxy)acrylate)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 2 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN



AN 2007:61333 CAPLUS Full-text
DN 146:162998
TI Preparation of 3-aminoazetidinecarboxamides as antagonists of sensory neuron specific (SNS) sodium channels
IN Hamlyn, Richard; Callis, David; Earnshaw, Christopher Geoffrey; Finch, Harry; Huckstep, Mike; Lynch, Rosemary; Mellor, Sarah
PA Vernalis (R & D) Limited, UK
SO PCT Int. Appl., 59pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2007007057 | A1 | 20070118 | WO 2006-GB2523 | 20060707 |

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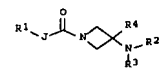
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI GB 2005-14017 A 20050707
OS MARPAT 146:162998
GI



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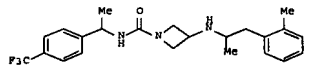
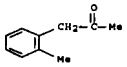


II

AB Title compds. I [wherein R1, R2 = (un)substituted Ph, heteroaryl, carbocyclyl, etc.; J = (un)substituted NH, O, or direct bond; R4, R3 = H, alkyl, alkenyl, etc.; R2 and R3 may link together to form ring] and pharmaceutically acceptable salts thereof were prepared as antagonists of sensory neuron specific (SNS) sodium channels. For instance, successive treatment of [1-[4-(trifluoromethyl)phenyl]ethyl]amine with 1,1'-carbonyl diimidazole, condensation with (azetidin-3-yl)carbamic acid tert-Bu ester (67% for two steps), deprotection with TFA (99%), and reductive alkylation with 2-methylphenylacetone (20%) gave azetidinecarboxamide II. This product showed inhibition of human Nav 1.8 stably expressed in SH-SY-5Y cells with an IC50



value of 1.30. Therefore, the invented compds. are useful for the treatment or prevention of a condition involving sodium ion flux through a sensory neuron specific channel of a sensory neuron, such as pain.
IT 51052-00-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aminoazetidinecarboxamides as antagonists of sensory neuron specific (SNS) sodium channels)
RN 51052-00-7 CAPLUS
CN 2-Propanone, 1-(2-methylphenyl)- (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

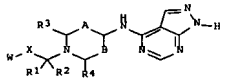
L31 ANSWER 3 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1124432 CAPLUS Full-text
DN 145:455026
TI N-alkyl-azacycloalkyl compounds as NMDA/NR2B antagonists and their preparation, pharmaceutical compositions, and use in the treatment of various diseases
IN Layton, Mark E.; Rodzinak, Kevin J.; Kelly, Michael J., III; Sanderson, Philip E.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 88pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2006113471 | A2 | 20061026 | WO 2006-US14139 | 20060414 |

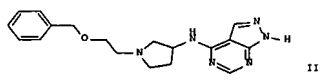
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI US 2005-672639P P 20050419
OS MARPAT 145:455026
GI



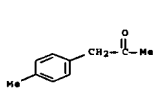


I



II

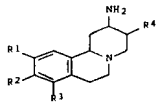
AB Compds. represented by formula I: and/or pharmaceutically acceptable salts, individual enantiomers and stereoisomers thereof, are effective as NMDA/NR2B antagonists useful for treating conditions such as pain, Parkinson's disease, Alzheimer's disease, epilepsy, depression, anxiety, ischemic brain injury including stroke. Compds. of formula I wherein W is (un)substituted (hetero)aryl; X is absent and (un)substituted C1-4 alkoxy and (un)substituted C1-3 alkyl; A is a bond and (un)substituted C2-3 alkyl, etc.; B is (un)substituted C1 alkyl, etc.; R1 and R2 are independently H and C1-3 alkyl; R3 and R4 are independently H, OH, CN and (un)substituted C1-3 alkyl, etc.; and their pharmaceutically acceptable salts, enantiomers and stereoisomers thereof are claimed. Example compound II was prepared by alkylation of tert-Bu pyrrolidin-3-ylcarbamate with [(2-bromoethoxy)methyl]benzene; the resulting tert-Bu [1-[2-(benzyloxy)ethyl]pyrrolidin-3-yl]carbamate underwent hydrolysis to give 1-[2-(benzyloxy)ethyl]pyrrolidin-3-amine, which underwent coupling with 4-chloro-1-(tetrahydropyran-2-yl)-1H- pyrazolo[3,4-d]pyrimidine to give compound II. All the invention compds. were evaluated for their NMDA/NR2B antagonistic activity.
IT 2096-86-8, (4-Methylphenyl)acetone
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of N-alkyl-azacycloalkyl as NMDA/NR2B antagonists useful in treatment of diseases)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



L31 ANSWER 4 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:517172 CAPLUS Full-text
DN 145:27873
TI Preparation of pyrido[2,1-a]isoquinolines as dipeptidyl peptidase IV (DPP-IV) inhibitors.
IN Boehringer, Markus; Hunziker, Daniel; Kuhn, Bernd; Loeffler, Bernd Michael; Ricklin, Fabienne; Wessel, Hans Peter

PA Awtz.
SO U.S. Pat. Appl. Publ., 41 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

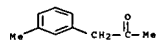
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | US 2006116393 | A1 | 20060601 | US 2005-288648 | 20051128 |
| | AU 2005311511 | A1 | 20060608 | AU 2005-311511 | 20051121 |
| | CA 2587524 | A1 | 20060608 | CA 2005-2587524 | 20051121 |
| | WO 2006058628 | A2 | 20060608 | WO 2005-EP12436 | 20051121 |
| | WO 2006058628 | A3 | 20060810 | | |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| | RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | IN 2007DN03795 | A | 20070824 | IN 2007-DN3795 | 20070522 |
| PRAI | EP 2004-106191 | A | 20041130 | | |
| | WO 2005-EP12436 | W | 20051121 | | |
| OS | MARPAT 145:27873 | | | | |
| GI | | | | | |



I

AB Title compds. [I; R1 = H, MeO; R2 = OH, (substituted) alkoxy, amino, aminocarbonylalkoxy, etc.; R3 = H, OH, (substituted) alkoxy, aminocarbonylalkoxy, amino, etc.; R4 = substituted Ph, pyridyl], were prepared Thus, (2SR,3SR,11bSR)-2-[2-amino-3-(2,5-dimethylphenyl)-10-methoxy-1,3,4,6,7,11b-hexahydro-2H-pyrido[2,1-a]isoquinolin-9-yloxy]acetamide hydrochloride (preparation from 9-benzyloxy-10-methoxy-1,3,4,6,7,11b-hexahydropyrido[1,2-a]isoquinolin-2-one given) inhibited DPP-IV with IC50 = 0.0001 μM.
IT 18826-61-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyridoisoquinolines as dipeptidyl peptidase inhibitors)
RN 18826-61-4 CAPLUS
CN 2-Propanone, 1-(3-methylphenyl)- (CA INDEX NAME)





L31 ANSWER 5 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:15022 CAPLUS Full-text
DN 144:108337
TI Preparation of pyridazine compounds as agrochemical fungicides
IN Morishita, Hiroshi; Manabe, Akio
PA Sumitomo Chemical Co., Ltd., Japan
SO PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

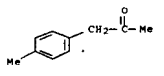
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2006001175 | A1 | 20060105 | WO 2005-JP10541 | 20050602 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| | RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | JP 2006045192 | A | 20060216 | JP 2005-158566 | 20050531 |
| | EP 1775290 | A1 | 20070418 | EP 2005-748513 | 20050602 |
| | R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR | | | | |
| PRAI | JP 2004-189396 | A | 20040628 | | |
| | WO 2005-JP10541 | W | 20050602 | | |
| OS | MARPAT 144:108337 | | | | |
| GI | | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1, R2 = alkyl; R3 = halo, nitro, cyano, etc.; m = 0-5; R4 = halo, nitro, cyano, etc.; R5 = halo, nitro, cyano, etc.; n = 0-4] were prepared For example, reaction of compound II, e.g., prepared from 2,4,6-trifluorobenzaldehyde in 3 steps, with hydrazine hydrate followed by in-situ treatment with PtO2 afforded compound III. In controlling test against Pyricularia oryzae, 10 examples of compds. I exhibited the fungicidal activity of ≥90%. Compds. I are claimed useful as agrochem. fungicides.
IT 2096-86-8, (4-Methylphenyl)acetone
RL: RCT (Reactant); RACT (Reactant or reagent)



(preparation of pyridazine compds. as agrochem. fungicides)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



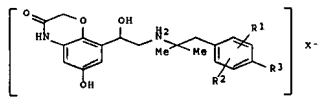
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 6 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:1224413 CAPLUS Full-text
DN 143:483127
TI Aerosol formulation for the inhalation of β-adrenoceptor agonists
IN Aven, Michael
PA Boehringer Ingelheim International GmbH, Germany
SO U.S. Pat. Appl. Publ., 23 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | US 2005256115 | A1 | 20051117 | US 2005-125756 | 20050510 |
| | DE 102004024452 | A1 | 20051208 | DE 2004-102004024452 | 20040514 |
| | AU 2005244414 | A1 | 20051124 | AU 2005-244414 | 20050510 |
| | CA 2564379 | A1 | 20051124 | CA 2005-2564379 | 20050510 |
| | WO 2005110421 | A2 | 20051124 | WO 2005-EP5028 | 20050510 |
| | WO 2005110421 | A3 | 20060316 | | |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| | RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | EP 1809293 | A2 | 20070725 | EP 2005-747843 | 20050510 |
| | R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR | | | | |
| | CN 101056640 | A | 20071017 | CN 2005-80015486 | 20050510 |
| | IN 2006DN06285 | A | 20070831 | IN 2006-DN6285 | 20061026 |
| | NO 2006005030 | A | 20061130 | NO 2006-5030 | 20061102 |
| | KR 2007022084 | A | 20070223 | KR 2006-726225 | 20061213 |
| PRAI | DE 2004-102004024452 | A | 20040514 | | |
| | US 2004-578541P | P | 20040610 | | |
| | WO 2005-EP5028 | W | 20050510 | | |
| | WO 2005-EP5078 | W | 20050511 | | |

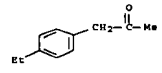


OS CASREACT 143:483127; MARPAT 143:483127
GI



I

AB The present invention relates to a propellant-free aerosol formulation of β-adrenoceptor agonists comprising one or more compds. of general formula I (R1,R2 = H, C1-4-alkyl, C1-4-alkoxy, halogen; R3 = H, C1-4-alkyl, C1-4-alkoxy, halogen, OH, O-C1-4-alkylene-CO2H, O-C1-4-alkylene-CO2-C1-4-alkyl; X- = anion), optionally in the form of their tautomers, enantiomers, mixts. of enantiomers, racemates or solvates, at least one pharmacol. acceptable acid, optionally other pharmacol. acceptable excipients and/or complexing agents, and, as solvent, water, ethanol or their mixture For example, (R)-6-hydroxy-8-[1-hydroxy-2-[2-(4-hydroxy-2,6-dimethylphenyl)-1,1-dimethylethylamino]ethyl]-4H-benzo[1,4]oxazin-3-one-methanesulfonate (II) was prepared and formulated into aerosol inhalant containing II 10 mg, benzalkonium chloride 10 mg, citric acid 3 mg, and water 100 mL.
IT 75251-24-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and aerosol formulation for inhalation of β-adrenoceptor agonists)
RN 75251-24-0 CAPLUS
CN 2-Propanone, 1-(4-ethylphenyl)- (9CI) (CA INDEX NAME)

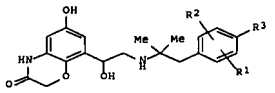


L31 ANSWER 7 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:1171119 CAPLUS Full-text
DN 143:440425
TI Preparation of benzoxazinone derivatives for treating respiratory tract diseases
IN Bouyssou, Thierry; Konetzki, Ingo; Pestel, Sabine; Schnapp, Andreas; Hoenke, Christoph; Lustenberger, Philipp; Rudolf, Klaus; Buettner, Frank; Heine, Claudia; et al.
PA Boehringer Ingelheim International GmbH, Germany; Boehringer Ingelheim Pharma GmbH & Co. KG
SO PCT Int. Appl., 54 pp.

CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2005102350 | A1 | 20051103 | WO 2005-EP4075 | 20050418 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| DE 102004019539 | A1 | 20051110 | DE 2004-102004019539 | 20040422 |
| AU 2005235420 | A1 | 20051103 | AU 2005-235420 | 20050418 |
| CA 2559700 | A1 | 20051103 | CA 2005-2559700 | 20050418 |
| EP 1765355 | A1 | 20070328 | EP 2005-740045 | 20050418 |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR | | | | |
| CN 1946406 | A | 20070411 | CN 2005-80012623 | 20050418 |
| BR 2005010084 | A | 20071016 | BR 2005-10084 | 20050418 |
| US 2005272726 | A1 | 20051208 | US 2005-109030 | 20050419 |
| MX 2006PA10577 | A | 20061110 | MX 2006-PA10577 | 20060915 |
| IN 2006DN05657 | A | 20070615 | IN 2006-DN5657 | 20060928 |
| NO 2006005061 | A | 20061107 | NO 2006-5061 | 20061102 |
| KR 2007054599 | A | 20070529 | KR 2006-724543 | 20061122 |
| PRAI DE 2004-102004019539 | A | 20040422 | | |
| US 2004-578569P | P | 20040610 | | |
| WO 2005-EP4075 | W | 20050418 | | |

OS MARPAT 143:440425
GI



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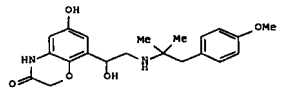
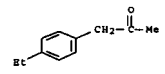


II



AB Title compds. I (R1 and R2 independently = H, halo, alkyl, etc.; R3 = alkyl, OH, halo, etc. with provisions) and their pharmaceutically acceptable salts, are prepared and disclosed as useful for treating respiratory tract diseases. Thus, e.g., II was prepared by coupling of 1,1-dimethyl-2-(4-methoxyphenyl)ethylamine with (6-benzyloxy)-4H-benzo[1,4]oxazin-3-one glyoxalhydrate followed by debenzylation. I should prove useful for the treatment of respiratory tract diseases such as but not limited to asthma, emphysema and adult respiratory distress syndrome. Pharmaceutical compns. comprising I are disclosed.
IT 75251-24-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzoxazinone derivs. for treating respiratory tract diseases)
RN 75251-24-0 CAPLUS
CN 2-Propanone, 1-(4-ethylphenyl)- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

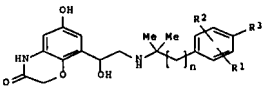
L31 ANSWER 8 OF 50 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:1155523 CAPLUS Full-text
DN 143:416252
TI Novel medicament combinations for the treatment of respiratory diseases
PA Boehringer Ingelheim International GmbH, Germany
SO U.S. Pat. Appl. Publ., 50 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI US 2005239778 | A1 | 20051027 | US 2005-109094 | 20050419 |
| DE 102004019540 | A1 | 20051110 | DE 2004-102004019540 | 20040422 |
| DE 102004052987 | A1 | 20060504 | DE 2004-102004052987 | 20041103 |
| AU 2005235419 | A1 | 20051103 | AU 2005-235419 | 20050418 |
| CA 2559699 | A1 | 20051103 | CA 2005-2559699 | 20050418 |
| WO 2005102349 | A1 | 20051103 | WO 2005-EP4073 | 20050418 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |



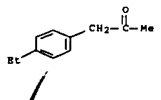
| | | | | |
|---|---|---|---|---|
| EP 1781298 | A1 | 20070509 | EP 2005-739576 | 20050418 |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR | | | | |
| CN 101035540 | A | 20070912 | CN 2005-80012621 | 20050418 |
| BR 2005010080 | A | 20071016 | BR 2005-10080 | 20050418 |
| MX 2006PA11721 | A | 20061211 | MX 2006-PA11721 | 20061010 |
| NO 2006005060 | A | 20061121 | NO 2006-5060 | 20061102 |
| KR 2007015592 | A | 20070205 | KR 2006-724528 | 20061122 |
| PRAI DE 2004-102004019540 | A | 20040422 | | |
| US 2004-578542P | P | 20040610 | | |
| DE 2004-102004052987 | A | 20041103 | | |
| EP 2005-2496 | A | 20050207 | | |
| WO 2005-EP4073 | W | 20050418 | | |

OS MARPAT 143:416252
GI



I

AB The present invention relates to a pharmaceutical compn. comprising one or more compds. of formula I wherein n denotes 1 or 2; R1 denotes hydrogen, halogen, C1-C4-alkyl or -O-C1-C4-alkyl; R2 denotes hydrogen, halogen, C1-C4-alkyl or -O-C1-C4-alkyl; R3 denotes C1-C4-alkyl, OH, halogen, -O-C1-C4-alkyl, -O-C1-C4-alkylene-COOH, -O-C1-C4-alkylene-CO- O-C1-C4-alkyl, and at least one other active substance for the treatment of respiratory diseases. The second active substance can by an anticholinergic, a phosphodiesterase IV inhibitor, a steroid, a LTD4 antagonist or an EGFR inhibitor.
IT 75251-24-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(novel medicament combinations for treatment of respiratory diseases)
RN 75251-24-0 CAPLUS
CN 2-Propanone, 1-(4-ethylphenyl)- (9CI) (CA INDEX NAME)



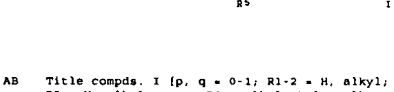
L31 ANSWER 9 OF 50 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:472128 CAPLUS Full-text
DN 143:26597
TI Preparation of substituted pyrazoles as PPARα and PPARγ agonists for treatment of dyslipidemia



IN Faucher, Nicolas Eric; Martres, Paul
PA Smithkline Beecham Corporation, USA
SO PCT Int. Appl., 176 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

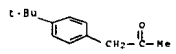
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2005049578 | A1 | 20050602 | WO 2004-EP12965 | 20041115 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1685113 | A1 | 20060802 | EP 2004-818779 | 20041115 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR, IS | | | | |
| JP 2007511485 | T | 20070510 | JP 2006-538823 | 20041115 |
| PRAI GB 2003-26747 | A | 20031117 | | |
| GB 2003-29462 | A | 20031219 | | |
| WO 2004-EP12965 | W | 20041115 | | |

OS MARPAT 143:26597
GI



I

AB Title compds. I [p, q = 0-1; R1-2 = H, alkyl; R3-4 = H, alkyl, alkoxy, etc.; R5 = H, alkyl, etc.; R6 = alkyl, halo, alkoxy, Ph, etc.] are prepared For instance, 2-[[4-[[[5-[4-(1,1-dimethylethyl)phenyl]-1-methyl-1H- pyrazol-3-yl]carbonyl]amino]methyl]-2-methylphenyl]oxy]-2-methylpropanoic acid (II) is produced in 7 steps from p-tert-Butylacetophenone, Et oxalate and methylhydrazine. II has EC50 = 0.014 μM for PPARα, 5.447 μM for PPARδ and 0.007 μM for PPARγ. I are useful in the treatment of diabetes, dyslipidemia or syndrome X.
IT 81561-77-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted pyrazoles as PPARα and PPARγ agonists for treatment of dyslipidemia)
RN 81561-77-5 CAPLUS
CN 2-Propanone, 1-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

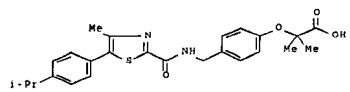


RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 10 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:371233 CAPLUS Full-text
DN 142:411351
TI Preparation of thiazole-2-carboxamide derivatives as hPPAR agonist
IN Gellibert, Francoise Joanne; Martres, Paul
PA Smithkline Beecham Corporation, USA
SO PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2005037804 | A1 | 20050428 | WO 2004-EP11386 | 20041007 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1680410 | A1 | 20060719 | EP 2004-790285 | 20041007 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR | | | | |
| JP 2007508270 | T | 20070405 | JP 2006-530145 | 20041007 |
| US 2007167628 | A1 | 20070719 | US 2007-575530 | 20070104 |
| PRAI GB 2003-23702 | A | 20031009 | | |
| WO 2004-EP11386 | W | 20041007 | | |

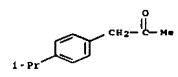
OS CASREACT 142:411351
GI



I

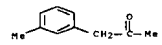


AB Title compound I and pharmaceutically acceptable salts thereof were prepared For example, acylation of Et 2-{[4-(aminomethyl)phenyl]oxy}-2-methylpropanoate with Et 4-methyl-5-[4-(1-methylethyl)phenyl]-1,3-thiazole- 2-carboxylate, e.g., prepared from 2,4-pentanedione in 4 steps, followed by hydrolysis using NaOH afforded compound I. In hPPARα binding assays, the EC50 value of compound I was 0.008 μM. Compds. I is claimed useful for the treatment of hypercholesteremia, heart failure, etc.
IT 7306-39-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thiazole-2-carboxamide derivs. as hPPAR agonist for treatment of hypercholesteremia, heart failure, etc.)
RN 7306-39-0 CAPLUS
CN 2-Propanone, 1-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 11 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:624095 CAPLUS Full-text
DN 142:335806
TI Product class 17: hydrazones
AU Kim, S.; Yoon, J.-Y.
CS Germany
SO Science of Synthesis (2004), 27, 671-722
CODEN: SSCYJ9
PB Georg Thieme Verlag
DT Journal; General Review
LA English
AB A review. Methods for preparing hydrazones and their application to organic synthesis are reviewed.
IT 18826-61-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and application of hydrazones to organic synthesis)
RN 18826-61-4 CAPLUS
CN 2-Propanone, 1-(3-methylphenyl)- (CA INDEX NAME)

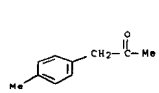


RE.CNT 188 THERE ARE 188 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 12 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN



AN 2004:580869 CAPLUS Full-text
DN 141:260346
TI Oxidative rearrangements of arylalkenes with [hydroxy(tosyloxy)iodo]benzene in 95% methanol: a general, regiospecific synthesis of α-aryl ketones
AU Justik, Michael W.; Koser, Gerald F.
CS Department of Chemistry, The University of Akron, Akron, OH, 44325-3601, USA
SO Tetrahedron Letters (2004), 45(32), 6159-6163
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
OS CASREACT 141:260346
AB The treatment of arylalkenes with [hydroxy(tosyloxy)iodo]benzene in 95% methanol affords the corresponding α-aryl ketones. This oxidative rearrangement is general for acyclic and cyclic arylalkenes and permits regioselective syntheses of isomeric α-Ph ketone pairs. For example, oxidative rearrangement of [1-(methylene)butyl]benzene gave 1-phenyl-2-pentanone. The oxidative rearrangement of (1-methyl-1- butenyl)benzene gave 3-phenyl-1-2-pentanone.
IT 2096-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of α-aryl ketones by oxidative rearrangement of (alkenyl)arenes in presence of [hydroxy(tosyloxy)iodo]benzene and methanol)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)

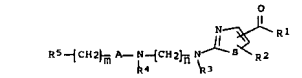


RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

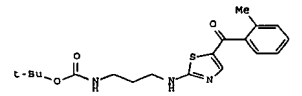
L33 ANSWER 13 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:696896 CAPLUS Full-text
DN 139:230771
TI Preparation of thiazoles as NPY receptor antagonists
IN Mattei, Patrizio; Neidhart, Werner; Nettekoven, Matthias Heinrich; Pflieger, Philippe; Taylor, Sven
PA F. Hoffmann-La Roche A.-G., Switz.
SO PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2003072577 | A1 | 20030904 | WO 2003-EP1667 | 20030219 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2475299 | A1 | 20030904 | CA 2003-2475299 | 20030219 |
| AU 2003210305 | A1 | 20030909 | AU 2003-210305 | 20030219 |
| EP 1480976 | A1 | 20041201 | EP 2003-742945 | 20030219 |
| EP 1480976 | B1 | 20070919 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| BR 2003008108 | A | 20041207 | BR 2003-8108 | 20030219 |
| CN 1639158 | A | 20050713 | CN 2003-804823 | 20030219 |
| JP 2005526732 | T | 20050908 | JP 2003-571283 | 20030219 |
| AT 373654 | T | 20071015 | AT 2003-742945 | 20030219 |
| US 2003225141 | A1 | 20031204 | US 2003-374573 | 20030226 |
| US 6686381 | B2 | 20040203 | | |
| MX 2004PA08379 | A | 20041126 | MX 2004-PA8379 | 20040827 |
| PRAI EP 2002-4296 | A | 20020228 | | |
| WO 2003-EP1667 | W | 20030219 | | |

OS MARPAT 139:230771
GI



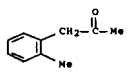
I



II

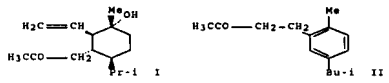
AB The title compds. (I; R1 = aryl, heteroaryl; R2-R4 = H, alkyl, cycloalkyl; R5 = alkyl, cycloalkyl, aryl, heteroaryl; R6 = H, alkyl, cycloalkyl; A = CO, SO2, NR6CO, OCO; n = 2-6; m = 0-2) which can be used in the form of pharmaceutical prepns. for the treatment or prevention of arthritis, cardiovascular diseases, diabetes, renal failure, eating disorders and obesity, were prepared and formulated. Thus, reacting 2-methylphenacyl bromide with tert-Bu [3-(3-dimethylaminomethylenethiourei do)propyl]carbamate (preparation given) in the presence of Et3N in EtOH afforded 77% II. Compds. I have IC50 values below 1000 nM against mNPY5. Most preferred compds. I have IC50 values below 10 nM (two examples given).
IT 51052-00-7
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of thiazoles as NPY receptor antagonists)
RN 51052-00-7 CAPLUS
CN 2-Propanone, 1-(2-methylphenyl)- (CA INDEX NAME)



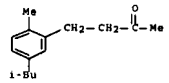
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 16 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:665514 CAPLUS Full-text
DN 139:377954
TI Two novel sesquiterpenes from the roots of Taiwania cryptomerioides Hayata
AU Kuo, Yueh-Hsiung; Chyu, Chiou-Feng
CS Department of Chemistry, National Taiwan University, Taipei, Taiwan, Peop. Rep. China
SO Tetrahedron Letters (2003), 44(38), 7221-7223
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science B.V.
DT Journal
LA English
GI



AB Two novel 3,4-secocadinane and 4,5-seco-8(7→6)-abeoguaiane skeletons, namely taiwaninones A (I) and B (II), together with khusinodiol and 4β,6β-dihydroxy-1α,5β(H)-guai-9-ene were isolated from the roots of Taiwania cryptomerioides. Their structures were elucidated by the spectral methods. The biotransformations of taiwaninones A and B were proposed from khusinodiol and 4β,6β-dihydroxy-1α,5β(H)-guai-9-ene, resp.
IT 623164-77-2P, Taiwaninone B
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(two novel sesquiterpenes from the roots of Taiwania cryptomerioides)
RN 623164-77-2 CAPLUS
CN 2-Butanone, 4-[2-methyl-5-(2-methylpropyl)phenyl]- (CA INDEX NAME)





RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

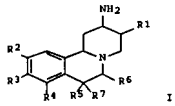
L1 ANSWER 15 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:532664 CAPLUS Full-text
DN 139:101038
TI Preparation of pyrido[2,1-a]isoquinoline derivatives as DPP-IV inhibitors
IN Gobbi, Luca Claudio; Luebbers, Thomas; Mattei, Patrizio; Narquizian, Robert; Wyss, Pierre Charles
PA F. Hoffmann-La Roche AG, Switz.
SO PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2003055881 | A1 | 20030710 | WO 2002-EP14685 | 20021220 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2003149071 | A1 | 20030807 | US 2002-321692 | 20021217 |
| US 6727261 | B2 | 20040427 | | |
| CA 2471262 | A1 | 20030710 | CA 2002-2471262 | 20021220 |
| AU 2002360074 | A1 | 20030715 | AU 2002-360074 | 20021220 |
| EP 1461337 | A1 | 20040929 | EP 2002-795262 | 20021220 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| BR 2002015396 | A | 20041207 | BR 2002-15396 | 20021220 |
| JP 2005518398 | T | 20050623 | JP 2003-556411 | 20021220 |
| CN 1639162 | A | 20050713 | CN 2002-826360 | 20021220 |
| HU 2006000068 | A2 | 20060529 | HU 2006-68 | 20021220 |
| NZ 533629 | A | 20060831 | NZ 2002-533629 | 20021220 |
| RU 2297417 | C2 | 20070420 | RU 2004-123215 | 20021220 |
| TW 265163 | B | 20061101 | TW 2002-91137130 | 20021224 |
| US 2004176406 | A1 | 20040909 | US 2004-800991 | 20040315 |
| US 6897222 | B2 | 20050524 | | |
| ZA 2004004926 | A | 20050913 | ZA 2004-4926 | 20040622 |
| MX 2004PA06241 | A | 20041101 | MX 2004-PA6241 | 20040623 |
| IN 2004CN01416 | A | 20060210 | IN 2004-CN1416 | 20040623 |
| NO 2004003174 | A | 20040726 | NO 2004-3174 | 20040726 |
| HK 1077069 | A1 | 20070706 | HK 2005-111787 | 20051221 |

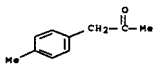


| | | | |
|---|---|---|---|
| PRAI EP 2001-130882 | A | 20011227 | |
| US 2002-321692 | A1 | 20021217 | |
| WO 2002-EP14685 | W | 20021220 | |

OS MARPAT 139:101038
GI



AB Pyridoisoquinolines I [R1 = alkyl, aryl, heteroaryl, aralkyl, heteroarylalkly, cycloakylalkyl; R2-R4 = H, halogen, OH, (un)substituted alkyl, alkoxy, alkenyl; R5 = H, F, alkyl, aryl; R6 = H, alkyl, hydroxyalkyl; R5R6 = atoms required to complete a 5- or 6-membered carbocyclic ring; R7 = H, F, alkyl] were prepared for use as DPP-IV inhibitors in the treatment of diseases, such as diabetes, particularly non-insulin dependent diabetes mellitus, and impaired glucose tolerance. Thus, 3,4-dihydro-6,7-dimethoxyisoquinoline was cyclized with AcOCHBuCH2N+Me3 I- to give the pyrido[2,1- a]isoquinolinone which was converted to its oxime and reduced with NiAl to give I [R1 = Bu, R2, R3 = OMe, R4-R7 = H, II]. 2α-II.2HCl had an IC50 for inhibition of DPP-IV of 0.52 μM.
IT 2096-86-8, 4-Methylphenylacetone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrido[2,1-a]isoquinoline derivs. as DPP-IV inhibitors)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

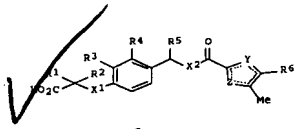
L1 ANSWER 18 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:927419 CAPLUS Full-text
DN 138:14053
TI Preparation of oxazoles and thiazoles as activators of the hPPARα receptor
IN Gellibert, Francoise Jeanne
PA Glaxo Group Limited, UK
SO PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DT Patent

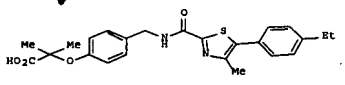


LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2002096895 | A1 | 20021205 | WO 2002-EP5886 | 20020529 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2448205 | A1 | 20021205 | CA 2002-2448205 | 20020529 |
| AU 2002317765 | A1 | 20021209 | AU 2002-317765 | 20020529 |
| EP 1399430 | A1 | 20040324 | EP 2002-747331 | 20020529 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| HU 2004000043 | A2 | 20040428 | HU 2004-43 | 20020529 |
| BR 2002009785 | A | 20040601 | BR 2002-9785 | 20020529 |
| JP 2004532267 | T | 20041021 | JP 2003-500074 | 20020529 |
| CN 1633421 | A | 20050629 | CN 2002-814942 | 20020529 |
| TW 245760 | B | 20051221 | TW 2002-91111392 | 20020529 |
| NZ 529754 | A | 20051223 | NZ 2002-529754 | 20020529 |
| ZA 2003009095 | A | 20050221 | ZA 2003-9095 | 20031121 |
| IN 2003KN01528 | A | 20060519 | IN 2003-KN1528 | 20031124 |
| MX 2003PA11032 | A | 20040319 | MX 2003-PA11032 | 20031128 |
| US 2005070517 | A1 | 20050331 | US 2004-478936 | 20040510 |
| US 7157479 | B2 | 20070102 | | |
| PRAI GB 2001-13231 | A | 20010531 | | |
| WO 2002-EP5886 | W | 20020529 | | |

OS MARPAT 138:14053
GI



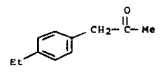


AB The title compds. [I; X1 = O, S; R1, R2 = H, alkyl; or R1 and R2 may together with the carbon atom to which they are bonded form a 3-5 membered cycloalkyl ring; R3, R4 = H, halo, Me, OMe; R5 = H, alkyl; X2 = NH, NMe, O; one of Y and Z is N, and the other is O or S; R6 = (un)substituted Ph or pyridyl (wherein the N is in position 2 or 3), with the provision that when R6 is pyridyl, the

N is unsubstituted], were prepared E.g., a multi-step synthesis of the acid II which showed EC50 of 5 nM against hPPARα binding, was given.

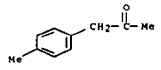
IT 75253-24-8, 4-Ethylphenylacetone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiazoles or oxazoles for the treatment of hPPARα mediated diseases)

RN 75251-24-0 CAPLUS
CN 2-Propanone, 1-(4-ethylphenyl)- (9CI) (CA INDEX NAME)



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 17 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:878889 CAPLUS Full-text
DN 136:278903
TI Reactions of aldehydes with polymer-supported selenoalkylidenetriphenylphosphoranes. A facile method for the synthesis of carbonyl compounds
AU Huang, Xian; Sheng, Shou-Ri
CS Xixi Campus, Department of Chemistry, Zhejiang University, Hangzhou, 310028, Peop. Rep. China
SO Tetrahedron Letters (2001), 42(51), 9035-9037
CODEN: TELEAY, ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 136:278903
AB The transylidation reactions of polymer-bound Se bromide with alkylidenetriphenylphosphoranes Ph3P:CHR (1) gave resin Ph3P:CR1Se-resin (2), which is sufficiently reactive to undergo Wittig-type reactions to afford the vinylic selenide resins R2CH:CR1Se-resin (3). Cleavage gave ketones R2CH2COR1 and aldehydes R2CH2CHO under different conditions.
IT 2096-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(reactions of aldehydes with polymer-supported selenoalkylidenetriphenylphosphoranes to give carbonyl compds.)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



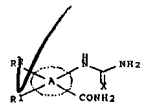


RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

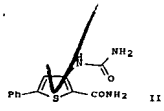
L31 ANSWER 18 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:597977 CAPLUS Full-text
DN 135:180698
TI Preparation of thiophenecarboxamides as inhibitors of the enzyme IKK-2
IN Baxter, Andrew; Brough, Stephen; Faull, Alan; Johnstone, Craig; Mcinally, Thomas
PA Astrazeneca AB, Swed.
SO PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2001058890 | A1 | 20010816 | WO 2001-SE248 | 20010207 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2396824 | A1 | 20010816 | CA 2001-2396824 | 20010207 |
| EP 1261600 | A1 | 20021204 | EP 2001-902951 | 20010207 |
| EP 1261600 | B1 | 20040506 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| BR 2001008143 | A | 20030121 | BR 2001-8143 | 20010207 |
| JP 2003522766 | T | 20030729 | JP 2001-558440 | 20010207 |
| AT 266019 | T | 20040515 | AT 2001-902951 | 20010207 |
| NZ 519947 | A | 20040528 | NZ 2001-519947 | 20010207 |
| PT 1261600 | T | 20040831 | PT 2001-902951 | 20010207 |
| ES 2218376 | T3 | 20041116 | ES 2001-1902951 | 20010207 |
| AU 781047 | B2 | 20050505 | AU 2001-30705 | 20010207 |
| US 2002107252 | A1 | 20020808 | US 2002-868884 | 20020205 |
| ZA 2002005300 | A | 20031002 | ZA 2002-5300 | 20020702 |
| NO 2002003786 | A | 20020923 | NO 2002-3786 | 20020809 |
| MX 2002PA07734 | A | 20021011 | MX 2002-PA7734 | 20020809 |
| PRAI GB 2000-3154 | A | 20000212 | | |
| WO 2001-SE248 | W | 20010207 | | |

OS MARPAT 135:180698
GI



I



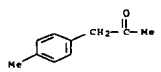
II



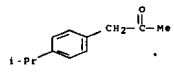
AB The title compds. [I; A = 5-membered heteroarom. ring containing 1-2 heteroatoms selected from O, N or S; R1 = (un)substituted Ph, 5-7 membered heteroarom. ring containing 1-3 heteroatoms selected from O, N or S; R2 = H, halo, CN, etc.; X = O, S], useful in the treatment or prophylaxis of inflammatory disease, were prepared Thus, refluxing 3-amino-5-phenyl-2-thiophenecarboxamide with trimethylsilyl isocyanate in DMF/CH2Cl2 afforded II.

IT 2096-86-8, (4-Methylphenyl)acetone 7306-39-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiophenecarboxamides as inhibitors of the enzyme IKK-2)

RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



RN 7306-39-0 CAPLUS
CN 2-Propanone, 1-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

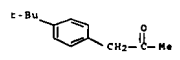
L31 ANSWER 19 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:775870 CAPLUS Full-text
DN 134:81972
TI Exploring the potential for allergic contact dermatitis via computed heats of reaction of haptens with protein end-groups: heats of reaction of haptens with protein end-groups by computation
AU Magee, Philip S.
CS BIOSAR Research Project, Vallejo, CA, 94591, USA
SO Quantitative Structure-Activity Relationships (2000), 19(4), 356-365
CODEN: QSARDI; ISSN: 0931-8771
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
AB Unlike human sensitization in allergic contact dermatitis, the primary event in the guinea pig maximization test (GPMT) is not penetration to the viable epidermis as the skin is compromised in both the sensitization and elicitation steps. The primary event is the chemical reaction of a hapten with simple protein end-groups at the recognition site of the major histocompatibility complex, class 2 (MHC II) on the cell surface of the Langerhans cells (LC). This reaction converts a benign LC into an allergen presenting cell that a T(CD4) lymphocyte recognizes as non-self and initiates the sensitizing



sequence in the local draining lymph node. The widely used GPMT was selected for the purpose of modeling the sensitizing reaction without the complications of penetration to the viable epidermis. The compds. selected for study represent the class of electrophilic haptens that, along with their metabolic precursors (prohaptens) comprise the majority of known contact allergens. As the whole MHC II structure has no involvement with the sensitizing reaction beyond the first few atoms of the end group, methoxide ion and thiomethoxide ion were used to model activated serine and cysteine. In addition, the GPMT has a relatively broad range of error which allows the use of AM1 as an adequate method for modeling the relative heats of reaction in the rate determining step. The relative reactivity of most of the known electrophilic haptens in the simplest aliphatic and aromatic form are modeled in this study. For many of those that are sensitive to substituent effects, sets of 7-10 substituted analogs were modeled to provide excellent Hammett relations with the heats of reaction. These linear free energy relations allow prediction of ACD potential in new related haptens. As a final validation of the procedure, a set of compds. scoring non , weak , moderate and strong as measured in the GPMT are computed for comparison with the test results and found to be in good concordance.

IT 81561-77-5
RL: ADV (Adverse effect, including toxicity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(exploring the potential for allergic contact dermatitis via computed heats of reaction of haptens with protein end-groups)

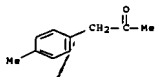
RN 81561-77-5 CAPLUS
CN 2-Propanone, 1-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



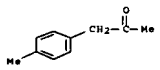
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 20 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:787486 CAPLUS Full-text
DN 132:40069
TI Determination and estimation of water solubility and n-octanol/water partition coefficient for substituted aromatic ketone and aldehyde
AU Ding, Yanbin; Cao, Jiasheng; Wang, Liansheng
CS State Key Laboratory of Pollution Control and Resource Reuse, Department of Environmental Sciences and Engineering, Nanjing University, Nanjing, 210093), Peop. Rep. China
SO Huanjing Huaxue (1999), 18(6), 543-546
CODEN: HUHUDB; ISSN: 0254-6108
PB Kexue Chubanshe
DT Journal
LA Chinese
AB Shake-flask method was used to determine water solubility (Sw) and n-octanol/water partition coefficient (Kow) for 15 substituted aromatic ketone and aldehyde. The result showed that the n-octanol/water partition coeffs. were correlated with water solubility Mol. connectivity indexes (MCIs) method has been used to established correlation equations. The estimated value were well fitted with observed
IT 2096-86-8, 2-Propanone 1-(4-methylphenyl)
RL: PRP (Properties)

(water solubility and n-octanol/water partition coefficient of substituted aromatic ketones and aldehydes)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



L33 ANSWER 21 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:572220 CAPLUS Full-text
DN 131:299277
TI The reaction of arylacetones with boron tribromide
AU Dupont, Romain; Cotelle, Philippe
CS Laboratoire Chimie Organique Physique, Univ. Lille, Villeneuve d'Ascq, F-59655, Fr.
SO Synthesis (1999), (9), 1651-1655
CODEN: SYNTBF; ISSN: 0039-7881
PB Georg Thieme Verlag
DT Journal
LA English
OS CASREACT 131:299277
AB Treatment of arylacetones with BBr3 gives 1,3-dimethyl-2- arylnaphthalenes in fair to good yields by a tandem aldol condensation-intramol. cyclization. This reaction is limited to the electron-rich arylacetones. In the case of (methoxyphenyl)acetones, a demethylation occurs leading to 1,3-dimethyl-2-(hydroxyphenyl)naphthols. Other cyclization may occur for (2-methoxyphenyl)acetones leading to an intramol. acetal or 5-, 6- or 7-hydroxy-2-methylbenzo[b]furans. In the case of 1-naphthylacetone, monobromination of the resulting phenanthrene occurs.
IT 2096-86-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(tandem aldol condensation-cyclization of arylacetones with boron bromide)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)

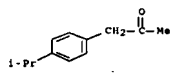


RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 22 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN



AN 1997:114551 CAPLUS Full-text
DN 126:171096
TI Enamine oxidations. 2. Selective oxidative cleavage of β,β-disubstituted enamines using alumina supported permanganate. Synthesis of one-carbon dehomologated carbonyl compounds from enamines
AU Harris, Clifford E.; Chrisman, William; Bickford, Sally A.; Lee, Lawrence Y.; Torreblanca, Antonia E.; Singaram, Bakthan
CS Department of Chemistry and Biochemistry, University of California, Santa Cruz, CA, 95064, USA
SO Tetrahedron Letters (1997), 38(6), 981-984
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
OS CASREACT 126:171096
AB Treatment of β,β-disubstituted enamines with potassium permanganate supported on neutral alumina leads to a mild and selective oxidative cleavage reaction which produces ketones and formamides. The ketones can be isolated in high yield and purity by a simple workup procedure. The oxidizing agent is selective and preferentially oxidizes an enamine carbon-carbon double bond in the presence of a distal carbon-carbon double bond. Other functional groups unaffected by this reagent include nitriles, secondary alcs., and alkynes allowing a wide range of potentially selective oxidns.
IT 7306-39-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(oxidative cleavage of β,β-disubstituted enamines using alumina supported permanganate)
RN 7306-39-0 CAPLUS
CN 2-Propanone, 1-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

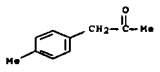


RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 23 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:414003 CAPLUS Full-text
DN 122:180432
TI Gas chromatographic determination of methamphetamine and its metabolite amphetamine in human plasma and urine following conversion to N-propyl derivatives
AU Jacob, Peyton III; Tisdale, Eileen Cotter; Panganiban, Kristina; Cannon, Dolores; Zabel, Karen; Mendelson, John E.; Jones, Reese T.
CS Drug Dependence Research Center, Langley Porter Psychiatric Institute, University of California, San Francisco, CA, 94143, USA
SO Journal of Chromatography, B: Biomedical Applications (1995), 664(2), 449-57
CODEN: JCBBEP; ISSN: 0378-4347
PB Elsevier
DT Journal
LA English



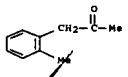
AB A gas chromatog. method for the simultaneous determination of methamphetamine and its metabolite amphetamine in human plasma and urine is described. The method utilizes reductive alkylation with propionaldehyde and sodium borohydride to produce N-Pr derivs., which have excellent chromatog. properties. Structural analogs of the analytes, p-methylmethamphetamine and p-methylamphetamine, are used as internal stds. The method has good precision and accuracy for concns. ranging from less than 10 ng/mL to 5000 ng/mL and has been used to measure plasma concns. as part of a pharmacokinetic/pharmacodynamic study of methamphetamine in humans.
IT 2096-86-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(methamphetamine internal anal. standard preparation)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



L33 ANSWER 24 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1992:5990 CAPLUS Full-text
DN 116:5990
TI Photocyclization of α-(o-tolyl)acetophenones: triplet and 1,5-biradical reactivity
AU Wagner, Peter J.; Meador, Michael A.; Zhou, Boli; Park, Bong Ser
CS Chem. Dep., Michigan State Univ., East Lansing, MI, 48824, USA
SO Journal of the American Chemical Society (1991), 113(25), 9630-9
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
OS CASREACT 116:5990
AB Several ring-substituted α-(o-tolyl)acetophenones undergo photocyclization to 2-indanol derivs. in high quantum efficiency in solution and in high chemical yield as solids. The mechanism for reaction involves triplet state δ-hydrogen atom abstraction that generates 1,5-biradicals. Quenching studies indicate that the n,π* excited triplets of these ketones react, with rate consts. >10⁸ s-1. Variations in triplet reactivity are ascribed to conformational equilibrium that populate reactive and unreactive geometries to different extents. The α-aryl ring eclipses the carbonyl in the lowest energy geometry, from which the most favorable geometry for reaction can be reached by small bond rotations. α-(2,4,6-Triisopropylphenyl)acetophenone forms the relatively long lived enol as well as indanol in solvent-dependent ratios; deuterium labeling indicates that the 1,5-biradical disproportionates to form enol. This does not happen with α-mesitylacetophenone, so its 54% cyclization quantum efficiency is ascribed to an internal triplet quenching that competes with hydrogen abstraction. This internal quenching is presumed to be of the charge-transfer type and does not appear to lead directly to 1,5-biradicals. 1-Methyl-2-phenyl-2-indanol is formed from α-(o-ethylphenyl)acetophenone with a Z/E ratio of 20:1 in benzene and 2:1 in methanol. The 1,5-biradical intermediates were characterized by flash spectroscopy; they have lifetimes



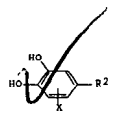
between 15 and 45 ns, with those derived from α-(o-isopropylphenyl) ketones being twice as long-lived as those derived from α-(o-methylphenyl) ketones, and show only a small solvent dependence. Biradical lifetimes and the diastereoselectivity of cyclization are interpreted in terms of biradical intersystem crossing occurring preferentially along the reaction coordinate for cyclization, such that the two processes effectively occur concurrently. The applicability of this concept to other biradicals is discussed. Authors counsel caution in addition of Br2 to DMF.
IT 51052-00-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 51052-00-7 CAPLUS
CN 2-Propanone, 1-(2-methylphenyl)- (CA INDEX NAME)



L33 ANSWER 25 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1991:655797 CAPLUS Full-text
DN 115:255797
TI Preparation and use of catechol derivatives as medical antioxidants
IN Korkolainen, Tapio Juhani; Nissinen, Erkki Aarne Olavi; Backstrom, Reijo Johannes; Pispuri, Aino Kyllikki
PA Orion-Yhtyma Oy, Finland
SO Eur. Pat. Appl., 14 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 4

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | EP 444899 | A2 | 19910904 | EP 1991-301587 | 19910227 |
| | EP 444899 | A3 | 19921125 | | |
| | EP 444899 | B1 | 19970205 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | JP 04211627 | A | 19920803 | JP 1991-30908 | 19910226 |
| | JP 3157846 | B2 | 20010416 | | |
| | AT 148626 | T | 19970215 | AT 1991-301587 | 19910227 |
| | HR 921250 | B1 | 20000630 | HR 1992-1250 | 19921112 |
| | US 5489614 | A | 19960206 | US 1995-461752 | 19950605 |
| PRAI | YU 1989-21 | A | 19890106 | | |
| | GB 1990-4348 | A | 19900227 | | |
| | FI 1986-4875 | A | 19861128 | | |
| | GB 1987-12437 | A | 19870528 | | |
| | US 1987-126911 | A3 | 19871127 | | |
| | US 1988-288979 | A2 | 19881223 | | |
| | US 1990-587791 | A2 | 19900925 | | |
| | US 1991-658666 | B1 | 19910221 | | |
| | US 1994-294762 | B1 | 19940823 | | |

OS MARPAT 115:255797
GI

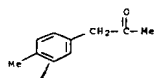


AB The title compds. [I; R2 = CH:CR3R4, CH2CHR3R4; R3 = acyl, cyclopropylcarbonyl; R4 = (un)substituted aryl, cyclopropylcarbonyl; X = halo, NO2, cyano, CF3, CHO, CO2H], their physiol. acceptable salts and esters, are claimed. Also claimed are the use of the known I (R2 = H, substituted alkyl, alkoxy, aryl, heterocyclyl, NO2, cyano, CHO, CO2H, CH:CR3R4, CH2CHR3R4; broader definitions for R3, R4 are given; X as above] and of their physiol. acceptable salts and esters for the prophylaxis and treatment of tissue damage induced in lipid peroxidn., e.g., in heart disease, rheumatoid arthritis, cancer, etc. Thus, a solution of Me2CHCOCH2Ph and 3,4,5-(HO)2(O2N)C6H2CHO in Me2CHOH was saturated by HCl(g) at 20° and stirred 4 h at room temperature to give title compound I (R2 = Me2CHCOCPh:CH, X = O2N). The latter in a controlled peroxidn. test in vitro had a stoichiometric factor 3.3 vs 2.0 for Trolox and 0.7 for ascorbic acid.

IT 2096-86-8, 3-(4-Methylphenyl)-2-propanone
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with (dihydroxy)nitrobenzaldehyde, in preparation
of medical antioxidants)

RN 2096-86-8 CAPLUS

CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



L31 ANSWER 26 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1991:152965 CAPLUS Full-text

DN 114:152965

TI Electrosynthesis of benzylic ketones

IN Robin, Yves; Chaussard, Jacques; Troupel, Michel; Guitton, Pascale

PA Societe Nationale des Poudres et Explosifs, Fr.

SO Fr. Demande, 27 pp.
CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI FR 2629474 | A1 | 19891006 | FR 1988-4254 | 19880331 |
| FR 2629474 | B1 | 19910412 | | |



PRAI FR 1988-4254 19880331

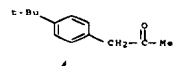
OS CASREACT 114:152965

AB Benzylic ketones are electrosynthesized from mixts. of an organic acid anhydride and a benzylic hetero compound chosen from benzylic quaternary ammonium salts, benzylic phosphonium compds., quaternary benzylic phosphonium compds., benzylic thiocyanates, and esters of benzylic alcs. more easily reducible than the anhydride. The anode, consumed in electrosynthesis, is chosen from Mg, Zn, Al, or their alloys. The process is easy and avoids use of benzylic halides. Application to pharmaceutical intermediates is indicated.

IT 81561-77-5P
RL: PREP (Preparation)
(electrosynthesis of)

RN 81561-77-5 CAPLUS

CN 2-Propanone, 1-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



L31 ANSWER 27 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1990:458690 CAPLUS Full-text

DN 113:58690

TI Method for oxidizing unsaturated aromatic compounds

IN Shimizu, Isoo; Matsumura, Yasuo; Iwamoto, Kouichi

PA Nippon Petrochemicals Co., Ltd., Japan

SO Eur. Pat. Appl., 10 pp.
CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI EP 350069 | A2 | 19900110 | EP 1989-112484 | 19890707 |
| EP 350069 | A3 | 19900530 | | |
| EP 350069 | B1 | 19930317 | | |
| R: CH, DE, FR, GB, IT, LI, SE | | | | |
| JP 02131435 | A | 19900521 | JP 1989-160324 | 19890622 |
| US 4967009 | A | 19901030 | US 1989-377183 | 19890707 |
| CA 1327607 | C | 19940308 | CA 1989-605013 | 19890707 |
| PRAI JP 1988-170577 | A | 19880708 | | |
| JP 1988-170578 | A | 19880708 | | |
| JP 1988-170579 | A | 19880708 | | |

OS MARPAT 113:58690

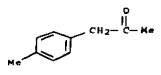
AB R1COCR2R3Ar (I; R1,R2,R3 = H, C1-4 alkyl, aryl; Ar = aryl) are prepared by oxidation of ArCR1:CR2R3 with an aryl iodosyl compound at -50° to 200°. MeCPh:CH2 (3 mmol) was treated with 3 mmol PhI(OAc)2 in 60% HOAc at 25° under N to give 26% PhCH2COMe with 30% conversion. Also prepared were 17 addnl. I. Other oxidizing agents were 4-MeC6H4IO, MeC6H4I(OBz)2, PhI(O2CCH2Cl)2, and 4-O2NC6H4IO.

IT 2096-86-8P, (4-Methylphenyl)acetone 64758-89-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 2096-86-8 CAPLUS

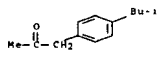
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)





RN 64758-89-0 CAPLUS

CN 2-Propanone, 1-[4-(2-methylpropyl)phenyl]- (9CI) (CA INDEX NAME)



L31 ANSWER 28 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1990:179438 CAPLUS Full-text

DN 112:179438

TI Facile nucleophilic addition of methyl ketone enolates to (η5-pentamethylcyclopentadienyl)rhodium η6-p-xylene dication

AU Fish, Richard H.; Kim, Hoon Sik; Fong, Raymond H.; Adams, Richard D.

CS Lawrence Berkeley Lab., Univ. California, Berkeley, CA, 94720, USA

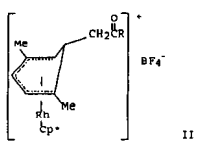
SO Organometallics (1990), 9(4), 1327-9
CODEN: ORGND7; ISSN: 0276-7333

DT Journal

LA English

OS CASREACT 112:179438

GI



II

AB The facile nucleophilic addition of Me ketone enolates of acetone, 2-butanone, and 2-pentanone to (η5-pentamethylcyclopentadienyl)rhodium (η6-p-xylene dication ([Cp*Rh(η6-1,4-Me2C6H4)2+], I) were studied by using 1,2,3,4-tetrahydroisoquinoline as the base at 25° to provide complexes II (R = Me, Et,

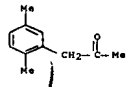


Pr), resp. The regio- and stereochem. of these ketone enolate addition reactions of I were established by a single-crystal x-ray structural anal. of the acetone enolate addition product, complex II (R = Me), to reveal that the substituted arene ligand, a 6-β-keto-substituted 1,4-dimethylcyclohexadienyl group, was bonded η5 to Cp*Rh+. The acetone enolate added to the unsubsciuted C position on the η6-p-xylene ligand of complex I by backside nucleophilic attack (exo to the Rh metal center). The scope of the reaction was briefly studied to show that only enolates of Me ketones were able to undergo this nucleophilic addition reaction to I. Complex II (R = Me) was oxidized with Jones reagent to release the 2,5-dimethylbenzyl Me ketone and provides a convenient synthetic method for this class of organic compds.

IT 53291-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from oxidation of rhodium complex)

RN 53291-89-7 CAPLUS

CN 2-Propanone, 1-(2,5-dimethylphenyl)- (9CI) (CA INDEX NAME)



L31 ANSWER 29 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1990:56295 CAPLUS Full-text

DN 112:56295

TI Allyl- and benzylstannanes, new reagents in terpenic synthesis

AU Andrianome, M.; Haberle, K.; Delmond, B.

CS Inst. Pin, Univ. Bordeaux 1, Talence, 33405, Fr.

SO Tetrahedron (1989), 45(4), 1079-88
CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

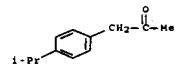
OS CASREACT 112:56295

AB Terpenic allyl- and benzylstannanes are easily prepared from unsatd. terpene hydrocarbons by metalation followed by quenching with trialkyltin chloride. An isomerization of unsatd. terpenes via allyltin compds. is reported, by which (+)-α-pinene was converted into (+)-β-pinene. Regioselective acylation of allyl- and benzylstannanes with acyl halides in the presence of rhodium catalysts gave mono- and sesquiterpenoid ketones which are important in the fragrance industry. Thus, treatment of 4-(Me2CH)C6H4CH2SnMe3 with senecioyl chloride in the presence of chlorotris(triphenylphosphine)rhodium gave 53% 4-(Me2CH)C6H4CH2COCH:CMe2.1. Hydroxylation and oxidation of terpene hydrocarbons via allyl- and benzylstannanes are also reported.

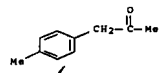
IT 7306-39-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 7306-39-0 CAPLUS

CN 2-Propanone, 1-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



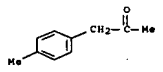
L34 ANSWER 30 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:134801 CAPLUS Full-text
DN 110:134801
TI Reagents and synthetic methods. 66. Reduction of α,β-unsaturated nitro compounds with tributyltin hydride
AU Aizpurua, J. M.; Oiarbide, M.; Palomo, C.
CS Fac. Cienc. Quim., Univ. Pais Vasco, San Sebastian, 20080, Spain
SO Tetrahedron Letters (1987), 28(44), 5365-6
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 110:134801
AB Reduction of R1C6H4CH:CRNO2 (I; R = H, Me; R1 = H, 4-Me, 4-Cl, 3-NO2, 4-OMe, 4-cyano) with Bu3SnH, followed by HF-MeOH work-up gave R1C6H4CH2CHRNO2. The reaction of I with Bu3SnH, followed by 3-ClC6H4CO2OH oxidation gave R1C6H4CH2COR via stannyl nitronates.
IT 2096-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



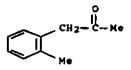
L34 ANSWER 31 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:94624 CAPLUS Full-text
DN 110:94624
TI Novel electrophilic species equivalent to α-keto cations. Reactions of 0,0-diprotonated nitro olefins with benzenes yield arylmethyl ketones
AU Okabe, Kazuaki; Ohwada, Tomohiko; Ohta, Toshiharu; Shudo, Koichi
CS Fac. Pharm. Sci., Univ. Tokyo, Tokyo, 113, Japan
SO Journal of Organic Chemistry (1989), 54(4), 733-4
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 110:94624
AB The N,N-dihydroxyiminium carbenium ions formed by O,O-diprotonation of nitro olefins in a strong acid, trifluoromethanesulfonic acid (TFSA), are discrete and novel dipositively charged species. The dications formed from α-substituted nitroethylenes are reactive electrophiles to give α-arylated



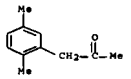
ketones in high yields. This constitutes a versatile synthetic method for the preparation of α-arylated ketones, which are difficult to synthesize by the conventional Friedel-Crafts reactions.
IT 2096-86-8P 51052-00-7P 53291-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



RN 51052-00-7 CAPLUS
CN 2-Propanone, 1-(2-methylphenyl)- (CA INDEX NAME)



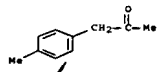
RN 53291-89-7 CAPLUS
CN 2-Propanone, 1-(2,5-dimethylphenyl)- (9CI) (CA INDEX NAME)



L34 ANSWER 32 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1988:437287 CAPLUS Full-text
DN 109:37287
TI Reagents and synthetic methods. 65. The Nef reaction of trialkylsilyl nitronates promoted by m-chloroperbenzoic acid. An efficient route to α-alkoxyketones from nitroalkanes
AU Aizpurua, J. M.; Oiarbide, M.; Palomo, C.
CS Fac. Cienc. Quim., Univ. Pais Vasco, San Sebastian, 20080, Spain
SO Tetrahedron Letters (1987), 28(44), 5361-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 109:37287



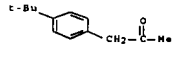
AB Treatment of 4-RC6H4CH2CHMeNO2 (R = H, Cl, Me, OMe, cyano) with Me3SiCl, followed by oxidation gave 92-99% yields 4-RC6H4CH2COMe, via trialkylsilyl nitronates. Other nitroalkanes reacted similarly to give alkoxyketones.
IT 2096-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



L34 ANSWER 33 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1987:466612 CAPLUS Full-text
DN 107:66612
TI An organic-electrolysis vat with a sacrificial electrode
PA Societe Nationale des Poudres et Explosifs, Japan
SO Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI JP 62056589 | A | 19870312 | JP 1986-208089 | 19860905 |
| FR 2586710 | A1 | 19870306 | FR 1985-13188 | 19850905 |
| FR 2586710 | B1 | 19900330 | | |
| EP 219367 | A1 | 19870422 | EP 1986-401895 | 19860829 |
| EP 219367 | B1 | 19900711 | | |
| R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE | | | | |
| AT 54472 | T | 19900715 | AT 1986-401895 | 19860829 |
| US 4686018 | A | 19870811 | US 1986-904025 | 19860902 |
| PRAI FR 1985-13188 | A | 19850905 | | |
| EP 1986-401895 | A | 19860829 | | |

AB An organic-electrolysis vat with a sacrificial electrodes is described, including uniquely designed electrodes to keep the spacing between the electrode constant A method for preparing a carboxylic acid, alc., ketone, or aldehyde by electrochem. reduction of an organic halide using the vat is also described.
IT 81561-77-5P
RL: PREP (Preparation)
(preparation of, electrochem.)
RN 81561-77-5 CAPLUS
CN 2-Propanone, 1-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

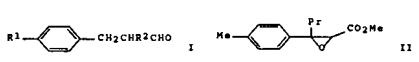




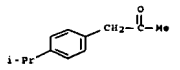
L37 ANSWER 34 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1987:32571 CAPLUS Full-text
DN 106:32571
TI 3-Phenylpropionaldehydes
IN Masso Ortigosa, Maria Teresa
PA Spain
SO Span., 29 pp.
CODEN: SPXXAD
DT Patent
LA Spanish
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI ES 541016 | A1 | 19851216 | ES 1985-541016 | 19850307 |
| PRAI ES 1985-541016 | | 19850307 | | |

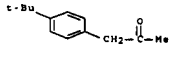
GI



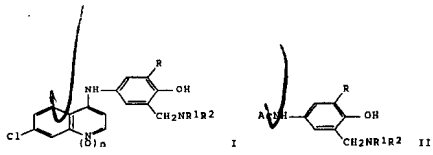
AB Title compds. I (R1 and R2 are alkyl) were prepared The Darzens condensation of 4-MeC6H4CH2COPr with ClCH2CO2Me in PhMe containing NaOMe gave glycidate ester II, and treatment of II with KOH gave I (R1 = Me, R2 = Pr).
IT 7306-39-0P 81561-77-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 7306-39-0 CAPLUS
CN 2-Propanone, 1-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 81561-77-5 CAPLUS
CN 2-Propanone, 1-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

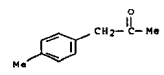


L31 ANSWER 35 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1986:207120 CAPLUS Full-text
DN 104:207120
TI Antimalarial drugs. 60. Synthesis, antimalarial activity, and quantitative structure-activity relationships of tebuquine and a series of related 5-[(7-chloro-4-quinolinyl)amino]-3-[(alkylamino)methyl][1,1'-biphenyl]-2-ols and N$\omega$-oxides
AU Werbel, Leslie M.; Cook, P. Dan; Elslager, Edward F.; Hung, Jocelyn H.; Johnson, Judith L.; Kesten, Stephen J.; McNamara, Dennis J.; Ortwine, Daniel F.; Worth, Donald F.
CS Warner-Lambert/Parke-Davis Pharm. Res., Ann Arbor, MI, 48105, USA
SO Journal of Medicinal Chemistry (1986), 29(6), 924-39
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 104:207120
GI

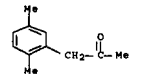



AB Title compds. I [n = 0, 1; R = (un)substituted Ph, 1-naphthyl, pyridyl; R1R2N = Et2N, adamantylamino, 1-pyrrolidinyl, etc.] were prepared from substituted 1-phenyl-2-propanones, proceeding through the 5-nitro[1,1'-biphenyl]-2-ols, the corresponding amino, and acetamido derivs. II and final condensation with 4,7-dichloroquinoline or the N-oxide. In a quant. structure-activity relationship study of 40 substituted Ph analogs and their N$\omega$-oxides, increasing antimalarial potency vs. Plasmodium berghei in mice was found to be correlated with decreasing size ($\Sigma$MR) and electron donation ($\Sigma$Es) of the Ph ring substituents. A significant correlation with N$\omega$-oxidation could not be demonstrated. Initial high activity against P. berghei infections in mice led to expanded studies that demonstrated in addition excellent activity against resistant strains of parasite, activity in primate models, and pharmacokinetic properties apparently allowing protection against infection for extended periods of time even after oral administration. Such properties encourage the clin. trial of a member of this class in man.
IT 2096-86-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitromalonaldehyde)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)





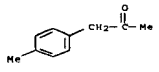

L31 ANSWER 36 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1985:45546 CAPLUS Full-text
DN 102:45546
TI A novel route to arylacetones via a masked $\alpha$-acylcarbonium intermediate
AU Shatzmiller, Shimon; Lidor, Ramy; Shalom, Eytan; Bahar, Eliezer
CS Dep. Chem., Tel-Aviv Univ., Tel Aviv-Jaffa, 69978, Israel
SO Journal of the Chemical Society, Chemical Communications (1984), (12), 795-6
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CASREACT 102:45546
AB Treatment of E- and Z-BrCH2CMe:NOMe with AgBF4 and five 1,3,4-RR1R2C6H3 (R, R2 = H, Me, OMe; R1 = H, OMe, OAc) in Cl(CH2)2Cl at 25° for 18 h in the dark gave the corresponding oxime ethers E-2,4,5-RR1R2C6H2CH2CMe:NOMe in 82-91% yield; subsequent acid hydrolysis with 1:5:5 HCl-H2O-MeOH at 65° for 10 h gave 2,4,5-RR1R2C6H2CH2COMe in 90% yield. E.g., 2,5-Me2C6H3CH2COMe was obtained from 1,4-Me2C6H4. The Ag+-induced aromatic substitution occurs via the acylcarbonium ion quiv. MeC(:NOMe)CH2+.
IT 53291-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53291-89-7 CAPLUS
CN 2-Propanone, 1-(2,5-dimethylphenyl)- (9CI) (CA INDEX NAME)



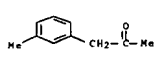

L31 ANSWER 37 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1984:173996 CAPLUS Full-text
DN 100:173996
TI Aromatic acetonylation promoted by manganese(III) and cerium(IV) salts
AU Kurz, Michael E.; Baru, Vijayalakshmi; Nguyen, P. Nhi
CS Dep. Chem., Illinois State Univ., Normal, IL, 61761, USA
SO Journal of Organic Chemistry (1984), 49(9), 1603-7
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 100:173996



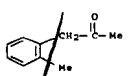
AB Treatment of aromatic hydrocarbons with Me2CO and Mn(OAc)3 gave arylacetones in yields from 26% with PhCl to 74% with PhOMe. Ce(IV) salts were also used successfully as promoters, but gave lower yields. The reactions were relatively free of side products except with PhMe. Isomer distributions, relative rates, and partial rate factors were determined for acetonylation of PhR (R = OMe, Me, Cl, F). A Hammett plot of the log of the partial rate factors for the Mn(III) system vs. $\sigma$-consts. gave a slope, $\rho$, of -2.4 ± 0.3. An isotope effect kH/kD of 3.8 was observed for the Mn(III)-promoted reaction with (CD3)2CO, indicating rate-determining proton loss from Me2CO. The overall mechanism involves formation and attack of acetonyl radical (I) on the aromatic hydrocarbon, followed by subsequent oxidative deprotonation of the resulting $\sigma$-radical complex. I exhibits appreciable electron-deficient character in its substitution behavior with aromatic hydrocarbons.
IT 2096-86-8
RL: PRP (Properties)
(isotope effect of, in aromatic acetonylations)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)




IT 18826-61-4P 51052-00-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 18826-61-4 CAPLUS
CN 2-Propanone, 1-(3-methylphenyl)- (CA INDEX NAME)




RN 51052-00-7 CAPLUS
CN 2-Propanone, 1-(2-methylphenyl)- (CA INDEX NAME)



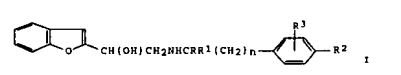

L31 ANSWER 38 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1982:544754 CAPLUS Full-text



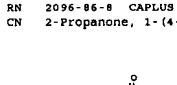
DN 97:144754
TI Secondary amines
IN Ferris, Michael John
PA Beecham Group Ltd., UK
SO Brit. UK Pat. Appl., 14 pp.
CODEN: BAXXDU
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | GB 2084577 | A | 19820415 | GB 1981-28824 | 19810923 |
| | GB 2084577 | B | 19840502 | | |
| | CA 1175851 | A1 | 19841009 | CA 1981-385953 | 19810915 |
| | ZA 8106567 | A | 19820929 | ZA 1981-6567 | 19810922 |
| | AU 8175603 | A | 19820401 | AU 1981-75603 | 19810923 |
| | AU 546104 | B2 | 19850815 | | |
| | EP 51917 | A1 | 19820519 | EP 1981-304398 | 19810923 |
| | EP 51917 | B1 | 19860219 | | |
| | R: BE, CH, DE, FR, IT, NL | | | | |
| | US 4432993 | A | 19840221 | US 1981-305117 | 19810924 |
| | JP 57085383 | A | 19820528 | JP 1981-151924 | 19810925 |
| | ES 505801 | A1 | 19830201 | ES 1981-505801 | 19810925 |
| PRAI | GB 1980-31228 | A | 19800926 | | |

OS CASREACT 97:144754; MARPAT 97:144754
GI



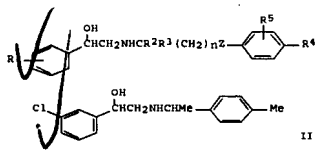

AB Benzofurylethanolamines I [R, R1 = H, Me; R2 = OH, (un)substituted alkoxy, alkyl; R3 = H, OH, halogen, alkyl, alkoxy; n = 1-3] were prepared Thus 2-formylbenzofuran was treated with Me3SiCN and reduced with LiAlH4 to give 2-(2-benzofuryl)-2-hydroxyethylamine which was treated with 4-MeC6H4CH2COMe and hydrogenated to give I (R = Me, R1 = R3 = H, R2 = Me, n = 1, II) as a mixture of diastereoisomers. II had antiobesity activity with only a slight effect on heart rate. Other I had antidiabetic, antiinflammatory, and platelet aggregation-inhibiting activity.
IT 2096-86-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzofurylethanolamine)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



L31 ANSWER 39 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1982:199276 CAPLUS Full-text
DN 96:199276
TI Arylethanolamine derivatives and their use in pharmaceutical compositions
IN Ferris, Michael John
PA Beecham Group Ltd. , UK
SO Eur. Pat. Appl., 62 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | EP 40000 | A1 | 19811118 | EP 1981-301606 | 19810413 |
| | EP 40000 | B1 | 19831012 | | |
| | R: BE, CH, DE, FR, GB, IT, NL, SE | | | | |
| | ZA 8102669 | A | 19820428 | ZA 1981-2669 | 19810423 |
| | JP 57002245 | A | 19820107 | JP 1981-68462 | 19810508 |
| | ES 502008 | A1 | 19830101 | ES 1981-502008 | 19810508 |
| | US 4588749 | A | 19860513 | US 1984-606597 | 19840503 |
| PRAI | GB 1980-15297 | A | 19800508 | | |
| | US 1981-257480 | A1 | 19810423 | | |

OS MARPAT 96:199276
GI



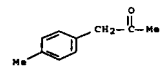
I



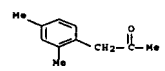
II

AB Ethanolamines I (R1 = H, F, Cl, Br, CF3, C1-4 alkyl; R2, R3 = H, C1-4 alkyl; R4 = C1-4 alkyl; R5 = H, C1-4 alkyl; n = 1-3; Z = O, bond), useful as hypoglycemics, antiinflammatory agents, and anti-obesity agents and having cardiac activity and effecting energy expenditure (extensive data given), were prepared Refluxing 4-MeC6H4CH2COMe with 3-ClC6H4CH(OH)CH2NH2 in C6H6 4 h, then hydrogenating the product gave diastereomeric ethanolamine II.
IT 2096-86-8 81561-61-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with ethanolamine derivs.)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)

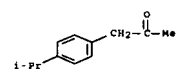




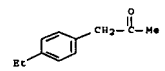
RN 81561-61-7 CAPLUS
CN 2-Propanone, 1-(2,4-dimethylphenyl)- (CA INDEX NAME)



IT 7306-39-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and condensation reaction of, with hydroxyphenethylamine)
RN 7306-39-0 CAPLUS
CN 2-Propanone, 1-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

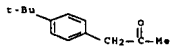


IT 75251-24-0P 81561-77-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with ethanamine derivative)
RN 75251-24-0 CAPLUS
CN 2-Propanone, 1-(4-ethylphenyl)- (9CI) (CA INDEX NAME)



RN 81561-77-5 CAPLUS
CN 2-Propanone, 1-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

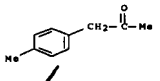




L31 ANSWER 40 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1982:162881 CAPLUS Full-text
DN 96:162881
TI Direct and retro processes of organometallic fragmentation. Part VI. Aromatization metalation as a method of synthesizing benzyl organometallic compounds containing an oxo group in the benzene ring
AU Rozenberg, V. I.; Nikanorov, V. A.; Reutov, O. A.
CS Inst. Elementoorg. Soedin., Moscow, USSR
SO Doklady Akademii Nauk SSSR (1981), 261(3), 637-41 [Chem.]
CODEN: DANKAS; ISSN: 0002-3264
DT Journal
LA Russian
GI

I

AB Treatment of PhCH2MgCl with AcCl in Et2O gave intermediate I which with HgCl2 in Et2O gave 12% 2-AcC6H4CH2HgCl. Similarly, p-MeC6H4CH2HgCl and AcCl in the presence of AlBr3 gave 25% 2,4-Ac(Me)C6H3CH2HgBr as the principal product in addition to p-MeC6H4CH2COMe and 2,5-Me2C6H3COMe. The mechanism of these processes were discussed.
IT 2096-86-8P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in acetylation of methylbenzylmercury halides by acetyl chloride)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



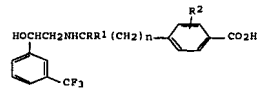
L31 ANSWER 41 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1982:162341 CAPLUS Full-text
DN 96:162341
TI Secondary amines and their use in pharmaceutical



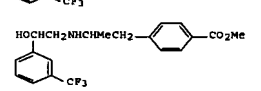
compositions
IN Ainsworth, Anthony Trevor; Smith, David Glynn
PA Beecham Group Ltd. , UK
SO Eur. Pat. Appl., 36 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | EP 40915 | A1 | 19811202 | EP 1981-301883 | 19810429 |
| | EP 40915 | B1 | 19840321 | | |
| | R: BE, CH, DE, FR, GB, IT, NL, SE | | | | |
| | CA 1181087 | A1 | 19850115 | CA 1981-377242 | 19810508 |
| | US 4385066 | A | 19830524 | US 1981-263168 | 19810513 |
| | ZA 8103203 | A | 19820526 | ZA 1981-3203 | 19810514 |
| | JP 57011949 | A | 19820121 | JP 1981-74327 | 19810519 |
| | AU 8170868 | A | 19811126 | AU 1981-70868 | 19810520 |
| | AU 539137 | B2 | 19840913 | | |
| | ES 502402 | A1 | 19830201 | ES 1981-502402 | 19810521 |
| | ES 516990 | A1 | 19831016 | ES 1982-516990 | 19821029 |
| PRAI | GB 1980-16890 | A | 19800522 | | |

OS MARPAT 96:162341
GI

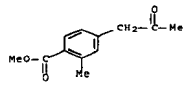


I

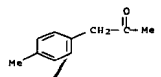


II

AB Amines I (R, R1 = H, Me; R2 = H, C1-6 alkyl, C1-6 alkoxy, halo; n = 1-3) were prepared as antiobesity agents, cardiac agents, hypoglycemics, and inflammation inhibitors. Thus, 3-(CF3)C6H4COCHO was treated with H2NCHMeCH2C6H4(CO2Me)-4 in refluxing C6H6 for 2 h and the resulting mixture was reduced by NaBH4 to give amine II as a 25:75 mixture of the RR,SS and RS,SR diastereoisomers. II at 10.5 mg/kg exhibited antiobesity activity in mice. Data are also given for the effect of I on energy expenditure in mice and for cardiac, hypoglycemic, and antiinflammatory activities of I.
IT 74733-50-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive amination of, with phenylethylamine derivative)
RN 74733-50-9 CAPLUS
CN Benzoic acid, 2-methyl-4-(2-oxopropyl)-, methyl ester (9CI) (CA INDEX NAME)



L1 ANSWER 42 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1982:115389 CAPLUS Full-text
DN 96:115389
TI Gas-chromatographic resolution of enantiomeric secondary alcohols. Stereoselective reductive metabolism of ketones in rabbit liver cytosol
AU Gal, Joseph; DeVito, Dino; Harper, Timothy W.
CS Sch. Med., Univ. Colorado, Denver, CO, 80262, USA
SO Drug Metabolism and Disposition (1981), 9(6), 557-60
CODEN: DMDSAI; ISSN: 0090-9556
DT Journal
LA English
AB A simple and rapid procedure suitable for the determination of the enantiomeric compns. of chiral alcs. (obtained by reductive metabolism of ketones such as methadone, adriamycin, etc.) extracted from biol. media is presented. The chiral alcs. were treated with (S)-(-)-1-phenylethylisocyanate [14649-03-7] and the resulting diastereomeric urethane derivs. were resolved on flexible fused silica capillary gas-liquid-chromatog. columns. The resolns. of the various carbinols were good to excellent. Alc. metabolites from rabbit liver supernatant fractions were determined with this procedure. The stereoselectivity of these redns. is presented and discussed.
IT 2096-86-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by liver, stereoselectivity of)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)

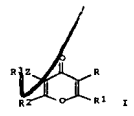


L1 ANSWER 43 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1981:83945 CAPLUS Full-text
DN 94:83945
TI 5-Substituted pyranone compounds for pharmaceutical uses
IN Clark, Barry Peter; Ross, William James; Todd, Alec
PA Lilly Industries Ltd., UK
SO Ger. Offen., 39 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1



| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | DE 3012597 | A1 | 19801016 | DE 1980-3012597 | 19800401 |
| | ES 490122 | A1 | 19810401 | ES 1980-490122 | 19800331 |
| | IL 59748 | A | 19831130 | IL 1980-59748 | 19800331 |
| | DK 8001421 | A | 19801006 | DK 1980-1421 | 19800401 |
| | FI 8001020 | A | 19801006 | FI 1980-1020 | 19800401 |
| | SE 8002515 | A | 19801006 | SE 1980-2515 | 19800401 |
| | AU 8057031 | A | 19801009 | AU 1980-57031 | 19800401 |
| | AU 535315 | B2 | 19840315 | | |
| | FR 2453168 | A1 | 19801031 | FR 1980-7447 | 19800402 |
| | FR 2453168 | B1 | 19830812 | | |
| | ZA 8001977 | A | 19810729 | ZA 1980-1977 | 19800402 |
| | AT 8001818 | A | 19820215 | AT 1980-1818 | 19800402 |
| | AT 368499 | B | 19821011 | | |
| | HU 25279 | A2 | 19830628 | HU 1980-785 | 19800402 |
| | HU 184257 | B | 19840730 | | |
| | CH 646967 | A5 | 19841228 | CH 1980-2589 | 19800402 |
| | BE 882644 | A1 | 19801003 | BE 1980-47126 | 19800403 |
| | GB 2047698 | A | 19801203 | GB 1980-11362 | 19800403 |
| | DD 150002 | A5 | 19810812 | DD 1980-220217 | 19800403 |
| | PL 123700 | B1 | 19821130 | PL 1980-223229 | 19800403 |
| | CA 1142944 | A1 | 19830315 | CA 1980-349145 | 19800403 |
| | NL 8002025 | A | 19801007 | NL 1980-2025 | 19800404 |
| | JP 55133376 | A | 19801017 | JP 1980-44550 | 19800404 |
| | CS 214826 | B2 | 19820625 | CS 1980-2358 | 19800404 |
| | SU 976850 | A3 | 19821123 | SU 1980-2905747 | 19800404 |
| | RO 81048 | A1 | 19830201 | RO 1980-100749 | 19800405 |
| | US 4364956 | A | 19821221 | US 1981-303307 | 19810917 |
| | GB 2123814 | A | 19840208 | GB 1983-12570 | 19830506 |
| | GB 2123814 | B | 19840801 | | |
| PRAI | GB 1979-12063 | A | 19790405 | | |
| | US 1980-134387 | A3 | 19800327 | | |
| | GB 1980-11362 | A | 19800403 | | |

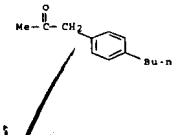
OS CASREACT 94:83945; MARPAT 94:83945
GI



AB The title compds. (I; R = H, alkyl, halogen; R1 = CO2R4, CONHR4, CN, 5-tetrazolyl, 5-tetrazolylcarbamoyl; R2,R4 = H, alkyl; R3 = optionally substituted Ph; Z = bond, O, S, SO, SO2) and their salts were prepared for use in treatment of allergies, especially asthma (no data). Thus, PhCH2COMe reacted with Me2NCH(OMe)2 to give Me2NCH:CPhCOMe, which was refluxed with (EtO2C)2 in EtOH-NaOEt to give I (R = R2 = H, R1 = CO2Et, R3Z = Ph).
IT 76512-42-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with DMF acetal, pyranone derivative from)
RN 76512-42-0 CAPLUS



CN 2-Propanone, 1-(4-butylphenyl)- (9CI) (CA INDEX NAME)



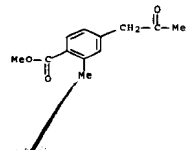
L1 ANSWER 44 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1981:15372 CAPLUS Full-text
DN 94:15372
TI Secondary amines and their use in pharmaceutical preparations
IN Ainsworth, Anthony Trevor; Smith, David Glynn
PA Beecham Group Ltd., UK
SO Eur. Pat. Appl., 89 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | EP 6735 | A1 | 19800109 | EP 1979-301197 | 19790621 |
| | EP 6735 | B1 | 19830615 | | |
| | R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE | | | | |
| | DK 7902727 | A | 19800204 | DK 1979-2727 | 19790627 |
| | CA 1159072 | A1 | 19831220 | CA 1979-330733 | 19790627 |
| | AU 7948498 | A | 19800103 | AU 1979-48498 | 19790628 |
| | AU 523681 | B2 | 19820812 | | |
| | JP 55009085 | A | 19800122 | JP 1979-82545 | 19790628 |
| | JP 01030820 | B | 19890622 | | |
| | ZA 7903231 | A | 19800730 | ZA 1979-3231 | 19790628 |
| | ES 483746 | A1 | 19800416 | ES 1979-483746 | 19790830 |
| | US 4478849 | A | 19841023 | US 1983-474199 | 19830310 |
| | ES 546425 | A3 | 19860201 | ES 1985-546425 | 19850731 |
| | US 4654371 | A | 19870331 | US 1985-785608 | 19851008 |
| | US 4753962 | A | 19880628 | US 1986-936714 | 19861201 |
| PRAI | GB 1978-28208 | | 19780628 | | |
| | GB 1978-46215 | | 19781127 | | |
| | US 1979-51440 | A1 | 19790625 | | |
| | US 1982-382379 | A3 | 19820527 | | |
| | US 1985-785608 | A1 | 19851008 | | |

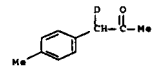
OS MARPAT 94:15372
GI



AB The title compds. I (R1 = H, F, Cl, OH, HOCH2, Me, MeO, H2N, HCONH, AcNH, MeSO2NH, O2N, PhCH2O, MeSO2CH2, H2NCONH, CF3, 4-MeOC6H4CH2NH; R2 = H, F, Cl, HO; R3 = H, Cl, HO; R4, R5 = H, Me, Et, Pr; R6 = CO2H, CONH2, CO2R where R = alkyl; R7 = H, Et, F, Me, MeO, HO, CO2H, CONH2, CO2R), useful as antidiabetics and in treatment of obesity (no data), were prepared Thus, 4-MeO2CC6H4CH2COMe refluxed with 4,3-HO(HOCH2)C6H4CH(OH)CH2NH2 followed by hydrogenation of the mixture gave II.
IT 74733-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with ethanamines)
RN 74733-50-9 CAPLUS
CN Benzoic acid, 2-methyl-4-(2-oxopropyl)-, methyl ester (9CI) (CA INDEX NAME)



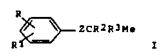
L1 ANSWER 45 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1978:189721 CAPLUS Full-text
DN 88:189721
TI Pull-push mechanism for the 1,2-hydrogen rearrangement of carbenes. Substituent and deuterium isotope effects for thermal decomposition of 1-phenyl-2-diazopropanes
AU Su, Dean T. T.; Thornton, Edward R.
CS Dep. Chem., Univ. Pennsylvania, Philadelphia, PA, USA
SO Journal of the American Chemical Society (1978), 100(6), 1872-5
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB Intramol. and intermol. D isotope effects in the rearrangement of carbenes generated from p-RC6H4CH2CMe:N2 (R = Me, H, Cl) and a Hammett treatment of the competition between benzylic and terminal H migration indicated a pull-push mechanism, which can be pictured roughly as electrophilic attack on the C-H bond by the phantom p orbital of the carbene along with backside nucleophilic attack by the carbene unshared electron pair to push the H away and form the π bond. The data are consistent only with a nonzero barrier for the carbene H rearrangement.
IT 66343-83-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and tosylhydrazone formation from)
RN 66343-83-7 CAPLUS
CN 2-Propanone-1-d, 1-(4-methylphenyl)- (9CI) (CA INDEX NAME)



L31 ANSWER 46 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1978:22392 CAPLUS Full-text
DN 88:22392
TI 4-Substituted butan-2-ones, but-3-en-2-ones, butan-2-ols, and but-3-en-2-ols and pharmaceutical compositions containing them
IN Cole, William Gwyn; Goudie, Alexander Crossan; Rose, Carl John
PA Beecham Group Ltd., UK
SO Brit., 17 pp.
CODEN: BRXXAA
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | GB 1479297 | A | 19770713 | GB 1974-29651 | 19740704 |
| | US 4062978 | A | 19771213 | US 1975-588638 | 19750620 |
| | US 4393079 | A | 19830712 | US 1976-750684 | 19761215 |
| | US 4216232 | A | 19800805 | US 1978-878675 | 19780217 |
| PRAI | GB 1974-29651 | A | 19740704 | | |
| | US 1975-588638 | A3 | 19750620 | | |
| | US 1975-599638 | A3 | 19750620 | | |
| | US 1976-750713 | A1 | 19761215 | | |

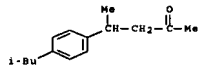
OS MARPAT 88:22392
GI



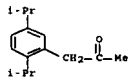
I

AB Nineteen title compds. I [R = 4-aroyl, -acyl, -alkyl, -allyloxy, -Ph, 3-PhO, -PhCO; R1 = H, 3-F, 4-MeO; Z = (CH2)2, CHMeCH2, CH:CH; R2R3 = O; R2 = H, R3 = OH] possess potent antiinflammatory activity but do not irritate the gastrointestinal tract to any major extent at the therapeutic dose when administered orally. Fourteen I were prepared, mainly by Friedel-Crafts acylation reactions or Cu-catalyzed alkylation. The antiinflammatory activities of I (R = 4-Ph, R2R3 = O)[R1 = H, 3-F, Z = CHMeCH2; R1 = H, Z = CH:CH, (CH2)2] were assessed in the carrageenan rat paw edema test; active doses were 30-33.3 mg/kg orally.
IT 65170-92-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(inflammation inhibitor, preparation of)
RN 65170-92-5 CAPLUS
CN 2-Pentanone, 4-[4-(2-methylpropyl)phenyl]- (9CI) (CA INDEX NAME)



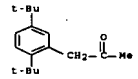


L31 ANSWER 47 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1976:73823 CAPLUS Full-text
DN 84:73823
TI Synthesis of arylacetones by the SRN 1 arylation of acetone enolate ion
AU Bunnett, Joseph F.; Sundberg, John E.
CS Univ. California, Santa Cruz, CA, USA
SO Chemical & Pharmaceutical Bulletin (1975), 23(11), 2620-8
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
DS CASREACT 84:73823
AB Numerous aryl bromides and iodides react with acetone enolate ion in liquid NH3 under irradiation to form arylacetones in high yield. This synthesis is successful with bromo- or iodobenzene derivs. carrying alkoxy, alkyl, phenyl, halogen, and carboxylate substituents, and with halogen derivs. of polynuclear aromatic hydrocarbons. The method is remarkably insensitive to steric hindrance; for example, 2,4,6-triethylbromobenzene reacts quite well. With greater steric hindrance, as in 2,4,6-triisopropyliodobenzene, reactivity falls and a side reaction of dehalogenation becomes appreciable. The synthesis was unsuccessful with the diethylamino, nitro and ionized hydroxy substituents. K-stimulated reactions of a few aryl diethyl phosphates with acetone enolate ion give generally lower yields of arylation and larger yields of dephosphation (hydrocarbon) products, compared even to K-stimulated reactions with aryl bromides. It is postulated that the lesser formation of hydrocarbon products from the aryl bromides is related to transport effects and solution inhomogeneity.
IT 58443-76-8P 58443-77-9P 58443-84-8P
58443-85-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 58443-76-8 CAPLUS
CN 2-Propanone, 1-[2,5-bis(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

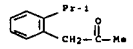


RN 58443-77-9 CAPLUS
CN 2-Propanone, 1-[2,5-bis(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

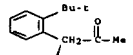




RN 58443-84-8 CAPLUS
CN 2-Propanone, 1-[2-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

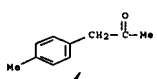


RN 58443-85-9 CAPLUS
CN 2-Propanone, 1-[2-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

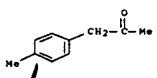


L31 ANSWER 48 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1974:520048 CAPLUS Full-text
DN 81:120048
TI New synthetic reactions. Regioselectivity and chemospecificity of the cyclopentane annulation-cyclopentenone annulation
AU Trost, Barry M.; Kurozumi, Seizi
CS Dep. Chem., Univ. Wisconsin, Madison, WI, USA
SO Tetrahedron Letters (1974), (22), 1929-32
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 81:120048
GI For diagram(s), see printed CA Issue.
AB Successive treatment of the oxaspiropentane I with LiN(CHMe2)2 in hexane and Me3SiCl followed by heating (330°) gave the cyclopentanone II. Use of Li pyrrolidide in place of LiN(CHMe2)2 gave the enol derivative III. Acid hydrolysis of III gave the cyclopentanone IV, successive bromination and dehydrobromination of III gave the cyclopentenone V.
IT 2096-86-8
RL: PROC (Process)
(cycloaddn. of, with cyclopropane derivative)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)





L31 ANSWER 49 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1972:72126 CAPLUS Full-text
DN 76:72126
OREF 76:11609a,11612a
TI Principle for establishing a carbon chain on an aromatic ring in place of nitrogen, oxygen, fluorine, sulfur, chlorine, bromine, or iodine functionality
AU Rossi, Roberto A.; Bunnett, J. F.
CS Univ. California, Santa Cruz, CA, USA
SO Journal of the American Chemical Society (1972), 94(2), 683-4
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB On reaction with K acetonate and K metal in liquid NH3 at -78°, PhNMe3+ I-, PhOP(O)(OEt)2, PhF, Ph2S, PhCl, PhBr and PhI give PhCH2Ac and PhCH2CH(OH)Me in (combined) yields of 46-89%. p-RC6H4Br and p-RC6H4NMe3+ I- (R = Me, MeO) similarly give (after oxidation) p-RC6H4CH2Ac. The method is of special interest because ArNMe3+ and ArOP(O)(OEt)2 (Ar = aryl) are easily made from ArNH2 and ArOH, resp.
IT 2096-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



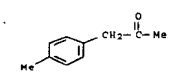
L31 ANSWER 50 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1968:505835 CAPLUS Full-text
DN 69:105835
OREF 69:19798h,19799a
TI 1,3-Dipolar cycloadditions on activated alkenes. II. Thermolysis of 3-cyano-3-ethoxycarbonyl-1-pyrazolines
AU Hamelin, Jack; Carrie, Robert
CS Fac. Sci. Rennes, Rennes, Fr.
SO Bulletin de la Societe Chimique de France (1968), (6), 2513-20
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA French
GI For diagram(s), see printed CA Issue.

AB I and II compds. are heated to give mixts. of Me(RCH2)C:C(CN)CO2Et (III), REtC:C(CN)CO2Et (IV), and V compds. Thus, I (R = p-MeOC6H4) is subjected to thermolysis to give 48% Et α-cyano-β-methyl-β-(p- methoxybenzyl)acrylate (VI), 18% Et α-cyano-β-ethyl-β-(p- methoxyphenyl)acrylate (VII), and 18% Et 2-methyl-2-(p-methoxyphenyl)-1- cyanocyclopropane (VIII). II (R = p-MeOC6H4) gives 78% VI, 5% VII, and 4% VIII. Also subjected to thermolysis are the following compds. (% III, % IV, and % V obtained given): I (R = p-ClC6H4), 36, 42, 25; II (R = p-ClC6H4), 88, 2, 7; I (R = Ph), 29, 41, 0; I (R = p-tolyl), 35, 35, 19; II (R = p-tolyl), 74, 6, 7; I (R = Et), 10, 52, 38; II (R = Et), 40, 24, 36; I (R = iso-Pr), 24, 42, 34; II (R = iso-Pr), 62, 12, 26. I (R = Me), or II (R = Me), gives 65% MeEtC:C(CN)CO2Et and 35% V (R = Me). N.M.R., ir, and uv data are given for the III (R = Ph, p-tolyl, p-ClC6H4, and p-MeOC6H4). The separation of VIII (b2-3 179-80°) and V (R = p-tolyl) (b2-3 169-71°) is described. Et 4-phenyl-4-benzyl-3-cyano-1- pyrazoline-3-carboxylate gives Ph(PhCH2CH2)C:C(CN)CO2Et, m. 95°. The following p-RC6H4CH2COMe compds. (R and b.p./mm. given): Cl, 82-4°/2-3; MeO, 100-2°/2; and Me, 138-40°/28; and VI (b0.5 175-7°), III (R = p-ClC6H4) (m. 54°), III (R = p-tolyl) (b0.1 138-40°), p-MeC6H4COEt (b2 70-2°), VII (m. 79-80°), IV (R = Ph), IV (R = p-ClC6H4) (m. .apprx.70°), and IV (R = p-tolyl) (b2 140°) are prepared according to known methods. Half-wave potentials are given for the III and IV, (Ar = Ph or a p-substituted Ph group).

IT 2096-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 2096-86-8 CAPLUS

CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



L31 ANSWER 51 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1960:34070 CAPLUS Full-text
DN 54:34070
OREF 54:6620c-d
TI A new method of preparation of o-tolylacetone
AU Konieczny, Mieczyslaw; Bobranski, Boguslaw
CS Akad. Med., Wroclaw, Pol.
SO Roczniki Chemii (1959), 33, 1027-30
CODEN: ROCHAC; ISSN: 0035-7677
DT Journal
LA English

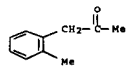
AB o-Cyanomethylbenzene (4.8 g.) in 5 g. dry EtOAc was added slowly to a boiling mixture of 4.6 g. Na butoxylate in 10 ml. anhydrous BuOH. The Na salt, precipitated at low temperature, was washed with Et2O, dissolved in H2O, and acidified with H2SO4 to obtain o-(acetylcyanomethyl)-toluene (I), b2 133-5°, yield 48%. I (1.46 g.) was heated with 6.4 ml. concentrated H2SO4 and 6 ml. H2O, extracted with Et2O, dried, and distilled to yield 76% o-tolylacetone, b3.5 87°; oxime m. 79-80°; 2,4-dinitrophenylhydrazone m. 145°.

IT 51052-00-7, 2-Propanone, o-tolyl-
(and derivs.)

RN 51052-00-7 CAPLUS



CN 2-Propanone, 1-(2-methylphenyl)- (CA INDEX NAME)



L31 ANSWER 52 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1951:55595 CAPLUS Full-text
DN 45:55595
OREF 45:9504g-i,9505a-d
TI Isomeric transformations of α-keto alcohols. VIII. Effect of a methyl group in the para position in a phenyl nucleus on the relative stability of isomeric alkaryl α-keto alcohols
AU Temnikova, T. I.; Petrova, L. A.
CS Leningrad State Univ.
SO Zhurnal Obshchei Khimii (1951), 21, 677-84
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Unavailable

AB cf. C.A. 44, 1056d, 4442f. Introduction of Me into the para position of Ph in alkaryl α-keto alcs. changes the properties of the substances by the inductive and mesomeric effects of the Me group. Of MeC6H4COCH(OH)Me and MeC6H4CHOHCOMe, the former is most stable. A saturated solution of 30 g. HCO2K in MeOH at 40° is treated with a 50% MeOH solution of p-MeC6H4CHBrAc (31 g. p-MeC6H4CH2Ac brominated and the crude product used directly) and stirred at gentle reflux 10 hrs. to yield 27% p-tolylacetylcarbinol (I), b1 100-1°, b1.5-2.0 103-6°, which on standing rapidly deposits a solid residue; semicarbazone, m. 189-90° (from EtOH); osasone, m. 141-3° (from EtOH). Treatment of the alc. with 2-3% MeOH-HCl yields the cyclodimethyldilactolide, C22H28O4, m. 253°. Attempts to prepare the carbinol by heating the Br ketone in a sealed tube with HCO2K at 110° gave tolylacetone and acetyldicoluyl, isolated as the disemicarbazone, m. 223-4° (decomposition, sealed tube). The solid m. 173°, formed on storage of the carbinol, has no OH groups, nor does it form a semicarbazone; possibly it is (p-MeC6H4CHAc)2O. Heating p-MeC6H4COCHBrMe with HCO2K and MeOH in a sealed tube 10 hrs. at 110° gave 37% product (II), b8 129-31°, b2 109-10°, b1 96°; semicarbazone, m. 188-9°, does not depress the m.p. of I semicarbazone; the yield of the semicarbazone indicates that the condensation yields a mixture of keto alcs. containing some 20-30% I. Treatment of the crude II with H2NCONHNH2 in aqueous MeOH, filtration of the precipitated semicarbazone, acidification of the filtrate with 5% H2SO4, warming on a steam bath, and extracting with Et2O gave methyl-p-toluylcarbinol cyclodimethyldilactolide, m. 230° (from C6H6-EtOH). Heating BzCl with crude II and BaCO3 failed to yield a Bz derivative, but heating 4 g. p-MeC6H4COCHBrMe and 4.2 g. BzOK in EtOH readily gave methyl-p- toluylcarbinyl benzoate, m. 96-9° (from ligroine). The isomerization of the 2 keto alcs. was followed by thermal analysis of their lolactolides. Crude II on this basis contains 20-5% I and 75-80% p-MeC6H4COCH(OH)Me (III). Heating this mixture (6.4 g.) 20 hrs. to 100° with fresh BaCO3 in a CO2 stream gave the cyclolactolide, m. 226°, corresponding to 90-5% III. Heating substantially pure I under similar conditions gave a cyclolactolide whose m.p. (227°) indicated 23-8% III concentration The cyclolactolide binary system has a min.

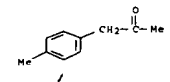


m.p. at about 210°, at approx. 40% I concentration The pure individual keto alcs. could not be isolated.

IT 2096-86-8P, 2-Propanone, p-tolyl-
RL: PREP (Preparation)
(preparation of)

RN 2096-86-8 CAPLUS

CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



L31 ANSWER 53 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1951:8882 CAPLUS Full-text
DN 45:8882
OREF 45:1626h-i,1627a-b
TI Ketones
IN Wolf, Anton
PA Knoll A.-G. Chemische Fabriken
DT Patent
LA Unavailable
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 752328 | | 19501003 | DE 1940-K159256 | 19401112 |

PI
GI For diagram(s), see printed CA Issue.

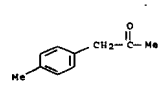
AB The process of preparing ketones by saponifying esters of α-alkyl- substituted β-(p-methoxyphenyl)glycidic acid in alkaline medium and splitting the resulting salts of the glycidic acid according to Ger. 727,045 is improved by use of esters O.CHR.CR'CO2R'' (I), of other α-alkyl-β-arylglycidic acids as initial material and by using organic acids instead of or as well as mineral acids to split the resulting salts. The ketones are useful as intermediates for the preparation of pharmaceuticals. Examples are given of the preparation of: benzyl Me ketone, b20 102-4°, from I (R = Ph, R' = Me; R'' is not specified); benzyl Et ketone, b15 116-18°, from I (R = Ph, R' = Et); m-methoxybenzyl Me ketone, b9 135-40°, from I (R = m-MeOC6H4, R' = Me); o-methoxybenzyl Me ketone, b10 127-30°, from I (R = o-MeOC6H4, R' = Me); 3,4-dimethoxybenzyl Me ketone (?), b7 170-5°, from I (R = 3,4(MeO)2C6H3, R' = iso-Pr); p-tolyl Me ketone (?), b8 108-12°, from II (R = p-MeC6H4, R' = Me). [The names of the last 2 compds. are apparently typographical errors for 3,4-dimethoxybenzyl iso-Pr ketone and p-methylbenzyl Me ketone, resp.-Abstractor.]

IT 2096-86-8P, 2-Propanone, p-tolyl-
RL: PREP (Preparation)
(preparation of)

RN 2096-86-8 CAPLUS

CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)





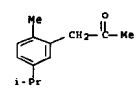
L31 ANSWER 54 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1950:30074 CAPLUS Full-text
DN 44:30074
OREF 44:5847i,5848a-b
TI Terpenes. VIII. The constitution of carotol. 3. A new synthesis of 1,7-dimethyl-4-isopropylnaphthalene
AU Sorm, F.; Mleziva, J.
SO Collection of Czechoslovak Chemical Communications (1949), 14, 98-107
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English

AB Carvone subjected to the Reformatskii reaction and followed by hydrolysis yielded carvacrylideneacetic acid, m. 112°, which, after boiling 6 hrs. with 100% HCO2H, rearranged to carvacrylacetic acid, m. 69°, which, converted to the acid chloride and treated with CdMe2, gave (2-p-cymyl)acetone, (I) b. 128°. I with Zn and BrCH2CO2Et, followed by treatment with HCO2H and alkaline hydrolysis, gave 3-(2-methyl-5-isopropylphenyl)-2-methyl-2-propene-1-carboxylic acid (II), b0.9 155-7°. During the above HCO2H treatment 20% I and EtOAc were also obtained. 3,5-Dimethyl-8-isopropyl-3,4-dihydro-1(2H)-naphthale-none (III) was obtained from the ring closure (by AlCl3) of the acid chloride of the hydrogenated form of II. III was reduced by LiAlH4 to the alc. which was dehydrogenated to 1,7-dimethyl-4- isopropylnaphthalene, m. 59°. The ultraviolet spectra, picrates, and styphnates of this synthetic sample and the one isolated from carotol (cf. C.A. 42, 7283b; 43, 3808b) were identical.

IT 96534-92-8P, 2-Propanone, carvacryl-
RL: PREP (Preparation)
(preparation of)

RN 96534-92-8 CAPLUS

CN 2-Propanone, carvacryl- (7CI) (CA INDEX NAME)



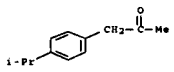
L31 ANSWER 55 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1948:2730 CAPLUS Full-text
DN 42:2730
OREF 42:602d-g
TI 1-Aryl-2-oxoalkanes
IN Tindall, John B.
PA Commercial Solvents Corp.

DT Patent
LA Unavailable
FAN.CNT 1

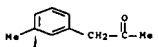
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 2427822 | | 19470923 | US 1945-600653 | 19450620 |

AB 1-Aryl-2-oxoalkanes are prepared by controlled catalytic hydrogenation of 1-aryl-2-nitro-1-alkenes and hydrolysis of the mixts. of arylnitroalkanes, aryloxoalkane oximes, and aryloxoalkanes so produced. The hydrogenation is effected with Pd or Pt in an inert solvent at 15-40° and 15-500 lb./sq. in., and the hydrolysis by treating first with alkali and then excess acid. Thus a mixture of MeC(NO2):CHPh 200, H2O 600, and 5% Pd on charcoal 2 parts was hydrogenated at 28-36° and 500 lb./sq. in. until H absorption practically ceased, and the filtered mixture was treated with NaOH 59 in H2O 500 parts at 65°, added to concentrated H2SO4 185 in H2O 1180 parts at 0-5°, and steam-distilled Distillation of the volatile oil gave 140.4 parts (85.3%) PhCH2COMe, b19 106-10°. Virtually the same procedure applied to EtC(NO2):CHPh 181.2 produced PhCH2COEt 94.5 parts (62%), b18 114-17°, n20 1.513, d2020 0.991, purity 98.3%. PrC(NO2):CHPh 149.8 similarly gave PhCH2COPr 88.2 parts (73.5%), b18 127-30°, n20 1.507, d2020 0.973, purity 100%. m-MeC6H4CH:C(NO2)Me 168 in MeOH 600 and 5% Pd on charcoal 3 parts hydrogenated at 20-21° and 300 lb./sq. in. and hydrolyzed essentially as before yielded m-tolylacetone 92 parts (65%), b18 118-19°. Like treatment of 1-p-cumyl-2-nitro-1-propene 142.7 parts in MeOH gave p-cumylacetone 67 parts (56%), b23 141-3°.

IT 7306-39-0P, 2-Propanone, p-cumenyl- 18826-61-4P, 2-Propanone, m-tolyl-
RL: PREP (Preparation)
(preparation of)
RN 7306-39-0 CAPLUS
CN 2-Propanone, 1-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



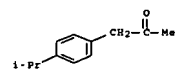
RN 18826-61-4 CAPLUS
CN 2-Propanone, 1-(3-methylphenyl)- (CA INDEX NAME)



L31 ANSWER 56 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1947:22349 CAPLUS Full-text
DN 41:22349
OREF 41:4471f-h
TI Synthesis of p-isopropyl-α-methylhydrocinnamaldehyde



AU Yamashita, Masataro
SO Bulletin of the Chemical Society of Japan (1941), 16, 413-16
CODEN: BCSJA8; ISSN: 0009-2673
DT Journal
LA Unavailable
AB Two new methods of synthesizing p-isopropyl-α- methylhydrocinnamaldehyde (I) from cuminyl chloride (II) have been devised. (1) II was converted into p-iso-PrC6H4CH2CN which was condensed with AcOEt in the presence of NaOEt to form p-iso-PrC6H4CH(COMe)CN and converted into p-iso-PrC6H4CH2COMe. The ketone and ClCH2CO2Et were again condensed to yield Et α,β-epoxy-γ-(p-isopropylphenyl)- β-methylbutyrate, which gave the desired I by saponification (2) II was converted by condensation with MeCHBrCH(OEt)2 into the di-Et acetal of I, which on hydrolysis with dilute HCl, yielded I.
IT 7306-39-0P, 2-Propanone, p-cumenyl-
RL: PREP (Preparation)
(preparation of)
RN 7306-39-0 CAPLUS
CN 2-Propanone, 1-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

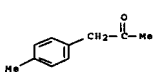


L31 ANSWER 57 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1946:3664 CAPLUS Full-text
DN 40:3664
OREF 40:606g-h
TI 4-Methylphenylacetone
IN Wenner, Wilhelm
PA Hoffmann-La Roche Inc.
DT Patent
LA Unavailable
FAN.CNT 1

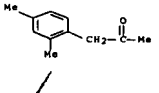
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 2382686 | | 19450814 | US 1942-43495442 | 19420316 |

AB A method of preparation of p-MeC6H4CH2Ac (I) involves the condensation of p-MeC6H4CH2CN (II) and AcOEt (III) and removal of the CN group from the resulting p-MeC6H4CH(CN)Ac (IV). A mixture of 131 g. II and 131 g. III is added to 30 g. Na in 300 g. absolute EtOH, refluxed for 2 h., hydrolyzed with H2O, and acidified with HOAc to give IV, b10 155-8°, m. 98°. IV (6 g.) is treated with 60 g. cold 80% H2SO4 and the mixture heated at 80-100° for 2 h., giving I, b10 104-6°. I (20 g.), in 50 g. of a 25% solution of MeNH2 in MeOH, hydrogenated at 90-100° over Raney Ni gives 1-(p-methylphenyl)-2-methylaminopropane, b10 105-6°; hydrobromide hemiethanolate, m. 159°.
IT 2096-86-8P, 2-Propanone, p-tolyl-
RL: PREP (Preparation)
(preparation of)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)





L31 ANSWER 58 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1939:41314 CAPLUS Full-text
DN 33:41314
OREF 33:5825c-f
TI Derivatives of 2,4-dimethylphenylacetic acid
AU Francais, Guy
SO Annali di Chimica Applicata (1939), 11, 212-43
CODEN: ACAPAR; ISSN: 0365-1037
DT Journal
LA Unavailable
AB The following ketones were prepared by the action of organo-Zn mixts. on 2,4-xylylacetyl chloride: 1-(2,4-dimethylphenyl)-2-propanone (I), 1-(2,4-dimethylphenyl)-2-butanone (II), 1-(2,4-dimethylphenyl)-2-pentanone (III), 1-(2,4-dimethylphenyl)-2-hexanone (IV), 1-(2,4-dimethylphenyl)-2- phenyl-2-ethanone, or 2,4-dimethyldesoxybenzoin (V), 1-(2,4- dimethylphenyl)-3-phenyl-2-propanone (VI). 1,3-Bis(2,4-dimethylphenyl)-2- propanone (VII) was prepared by the catalytic method of Senderens (C. A. 7, 1882) as was I and II. Pseudocumene formed during the latter reaction confirms the formula attributed to xylylacetic acid by Claus and Klocke (Ber. 19, 230 (1886)). Semicarbazones and oximes of the ketones mentioned above were prepared 2,4-Dimethylphenylhexane was produced by direct reduction of IV. Catalytic hydrogenation of the oxime of II (with Raney Ni) yielded the corresponding primary amine. Similarly, I, II, III, IV and V were reduced to the corresponding secondary alcs., of which derivs. with NH2CONHCO2H were prepared The rate of catalytic reduction diminishes with the length of the aliphatic chain containing the CO group. 2,4-Dimethylstilbene, C16H16, was prepared by saturating the carbinol resulting from the reduction of V with HBr and subsequently treating with excess K alcoholate.
IT 81561-61-7P, 2-Propanone, (2,4-xylyl)-
RL: PREP (Preparation)
(preparation of)
RN 81561-61-7 CAPLUS
CN 2-Propanone, 1-(2,4-dimethylphenyl)- (CA INDEX NAME)



L31 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1932:44518 CAPLUS Full-text
DN 26:44518
OREF 26:4592i,4593a-i,4594a-i,4595a-i
TI Polyterpenes and polyterpenoids. LXIV. Synthesis of sapotalene and other



trimethylnaphthalenes
AU Ruzicka, L.; Ehmann, L.
SO Helvetica Chimica Acta (1932), 15, 140-62
CODEN: HCACAV; ISSN: 0018-019X
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB In order to determine the constitution of trimethylnaphthalenes it is sometimes necessary to synthesize the compds. themselves since the m. p. of mixts. is not depressed sufficiently to be significant. R. and E. have undertaken to synthesize all the unknown trimethylnaphthalenes to accumulate data on the m. p. of mixts. of picrates and of styphnates. The following mixed picrates show significant depression of m. p.: 1,3,5 (140°) and 1,3,7 (142°), 135-7°; 1,3,7 and 1,2,3 (142.5°), 124-8°; 1,3,5 and 1,2,3, 136-7°; 1,3,5 and 1,4,5 (144.5°), 136-9°; 1,3,7 and 1,4,5, 131-3°; 1,2,6 (120.5°) and 2,3,5 (122.5°), 114-6°; 2,3,5 and 1,3,8 (122°), 113-8° 1,2,7 (129°) and 2,3,6 (130°), 115-23°; 2,3,6 and 1,2,8(133°),113-20°; 1,2,7 and 1,2,8, 123-5°. The following mixed picrates show little or no depression of m. p.: 1,4,6 (133°) and 1,2,5 (137.5°), 132-4°; 1,2,5 and 1,3,5, 134-7°; 1,2,3 (142.5°) and 1,4,5, 142-4°; 1,4,5 and 1,2,4 (147.5°), 144-6°; 1,2,3 and 1,2,4, 142-3°; 1,2,6 and 1,3,8, 121-2°. The mixed styphnates 1,2,4 (123.5°) and 1,4,5 (129.5°) show only a slight lowering of the m. p., 121-3°; in all others the lowering is significant: 1,2,8 (144.5°) and 2,3,5 (146.5°), 130-1°; 2,3,5 and 1,2,6 (148°), 132-5°; 1,2,6 and 1,3,7 (151.5°), 134-6°; 1,3,7 and 1,2,7 (156°), 144-5°; 1,2,8 and 1,2,6, 128-9°; 2,3,5 and 1,3,7, 132-3°; 1,2,8, and 1,3,7, 130-5°; 1,2,3 (143.5°) and 1,2,8, 127-30°; 1,2,3 and 2,3,5, 131-4°; 1,3,8((138°) and 1,3,5 (136.5°), 126-8°; 1,4,5 and 1,2,5 (129.5°), 116-9°; 1,2,4 and 1,2,5, 115-7°; 1,3,6 (126°) and 1,2,4, 110-4°; 1,3,6 and 1,4,5,106-10°; 1,4,6(114°) and 1,2,4, 111-6°. The following picrates are distinctively colored: 1,2,3, bright orange-yellow; 2,3,6,orange-yellow; 1,4,6, bright red-orange; 1,2,8,red-orange; 1,4,5, deep red-orange. Distinctively colored styphnates are: 2,3,6, canary-yellow; 1,3,5, lemon-yellow; 1,2,7, bright yellow; 1,2,6, yellow; 2,3,5, gold-yellow; 1,3,7, gold-orange; 1,2,4, yellow-orange; 1,4,5, red-brown. Preparation of 1,2,3-trimethyl- naphthalene (I) (WITH E. KELLER AND H. SCHUTZE): MeCOCH2Ph is condensed with MeCHBrCO2Et (II) to give a mixture of HO and unsatd. esters, b18 147-65°, which is changed in the usual way to Et γ-phenyl-α,β-dimethylcrotonate, PhCH2CMe: CMeCO2Et (III), b12, 143-6°. III is reduced catalytically (Pt) to Et α,β-dimethyl-γ-phenylbutyrate, b12 141-4°, which is saponified to α,β-dimethyl-γ-phenylbutyric acid (IV), b1.5 140-50°. Under the action of AlCl3, the acid chloride of IV, b12 130-40°, goes to 2,3-dimethyl-1-keto-1,2,3,4- tetrahydronaphthalene(V), b13 125-30°. V is treated with MeMgI to give an oil (VI), b12 120° (approx.), which consists mostly of the product formed by splitting off H2O from the tertiary alc. Through dehydrogenation, VI → I, b12 125-30°. I was also prepared (WITH P. PARODI-DELFINO) by the following reactions: PhCMe:CMeCO2Et (VII) is reduced catalytically to Et α-methyl-β-phenylbutyrate, b11 124-8°, which is saponified to the acid (VIII). b12 160-3°. The acid chloride of VIII, b12 117-20°, when treated with MeZnI in Et2O gives 80% of α-methyl-β-phenylpropyl Me ketone (IX), b11 115-7°. IX isreduced with Na and absolute EtOH to 3-methyl-4-phenyl-2- pentanol, b11 129-31°, which upon heating with 40% HBr-AcOH gives 25%, 2-bromo-3-methyl-4-phenylpentane (X), b11 128-30°. 2-Cyano-3-methyl-4-phenylpentane (XI). b11 132-8°, prepared from X when saponified with KOH in MeOH at 150° gives α,β-dimethyl- γ-phenylvaleric acid (XII), b10 172-4°. XII can also be prepared by the following reactions: IX + ClCH2CO2Et → Et δ-phenyl-β,γ-dimethyl-α,β-oxidocaproate, PhMeCHCHMe CMe.O.CHCO2Et, b10 162-3°,→ α, β-dimethyl-γ-phenylvaleraldehyde, b10 130-40°, → XII. I can be prepared from XII through 1,2,3-trimethyl-4-keto-1,2,3,4- tetrahydronaphthalene, but this synthesis was

not carried out because of poor yields of X and XI. Preparation of 1,2,4-trimethylnaphthalene (XIII) (WITH F. DES TOMBE AND H. RAMONDT): BzMe + II → VII → 2-methyl-3-phenyl-1-butanol (XIV) → 1-bromo-2-methyl-3- phenylbutane, (XV) → 1-cyano-2-methyl-3-phenylbutane (XVI) → β-methyl-γ-phenylvaleric acid (XVII) → β-methyl-γ-phenylvaleryl chloride (XVIII) → 1,2-dimethyl-4-keto-1,2,3,4-tetrahydronaphthalene (XIX) → 1,2,4-trimethyl-1,2-dihydronaphthalene (XX) → XIII. VII (C. A. 8, 1113) is reduced by the Bouveault reaction (Na in absolute EtOH) to XIV, b11 123-4°. XIV reacts with HBr-AcOH to give XV, b12 122°. XV + KCN in aqueous EtOH → XVI, which is saponified directly to XVII, b12 172°. XVIII, b12 132-3°, under the action of AlCl3 closes the ring to give XIX, b12 141°, which when treated with MeMgI goes directly to XX, b11 109°. XX heated with its own weight of Se for 30 hrs. at 320° is dehydrogenated to XIII, which, after 2 distns. over Na, b12 146°, recrystd. from MeOH (platelets), m. 50°. Preparation of 1,2,6-trimethylnaphthalene (XXI) (WITH J. CUENAT AND S. BIASUTTI): p-MeC6H4CMe: CMeCO2Et2 → 2-methyl-3-(p-tolyl)-1-butanol (XXII) → 1-bromo-2-methyl-3-(p-tolyl)butane (XXIII) → 1-cyano-2-methyl-3-(p-tolyl)butane (XXIV) → β-methyl-γ- (p-tolyl)valeric acid, p-MeC6H4MeCHMeCHCH2CO2H (XXV) →-methyl- β-(p-tolyl)valeryl chloride((XXVI) → 1,2,6-trirmethyl-4-keto- 1,2,3,4-tetrahydronaphthalene (XXVII) → 1,2,6-trimethyl-4-hydroxy- 1,2,3,4-tetrahydronaphthalene (XXVIII) → XXI. XXII, b12 132-6° (prepared by the Bouveault reaction), reacts with HBr-AcOH to give XXIII, b13 138-40°. XXIV is saponified to XXV, b11 188°, by heating in an autoclave at 150°. Ring closure of XXVI, b10 144°, using AlCl3 in CS2, gives XXVII, b10 153°, which is reduced to XXVIII, b10 133-4°, by Na in EtOH. Dehydrogenation of XXVIII with Se yields XXI, b10 146°. Preparation of 1,2,7-trimethylnaphthalene (XXIX), sapotalene (XXX) (with Ad. Renold): p-MeC6H4CH2CO2Et (XXXI) → β-(p-tolyl)-ethanol (XXXII) → β-(p-tolyl)ethyl bromide (XXXIII) → (+NaMeC(CO2Et)2) (XXXIV) → di-Et [β-(p-tolyl)ethyl]methylmalonate (XXXV) → α-methyl-γ-(p-tolyl)-butyric acid, p-MeC6H4(CH2)2CHMeCO2H (XXXVI) → α-methyl-γ-(p-tolyl)butyryl chloride (XXXVII)) → 2,7-dimethyl-1-keto-1,2,3,4-tetrahydronaphthalene (XXXVIII) → 1,2,7-trimethyl-3,4-dihydronaphthalene (XXXIX) → XXIX. XXXII, b14 117-8°, prepared by the reduction of XXXI with Na in absolute EtOH, when heated with 3 times its weight 33% HBrAcOH for 24 hrs. at 100° → XXXIII, b16 116°. XXXIII (52 g.) and the XXXIV from 64 g. MeCH(CO2Et)2 are boiled under reflux in C6H6; yield 66 g. XXXV, b16 191-3°. Saponification and decarboxylation of XXXV gives XXXVI, b13 172°, b18 188°, m. 50°, platelets from AcOEt. XXXVI (40 g.) and 50 g. SOCl2 are heated until the evolution of gases ceases and then distilled directly in vacuo; yield 40.7 g. XXXVII, b15 142°. XXXVII (35.7 g.) and 50 g. AlCl3 are heated in CS2 as long as HCl is evolved, giving 27.6 g. (92.5% yield) of XXXVIII, b13 142°, b18 153°. The semicarbazone of XXXVIII m. 218°. XXXVIII is heated 4 hrs. with an excess (2 mols.) of MeMgI. After several distns. of the reaction product over I, with a final distillation over Na, XXXIX is obtained, b13 130°. XXXIX is heated with twice its weight of Se 48 hrs. at 285° to dehydrogenate to XXIX, which is extracted with Et2O and distilled over Na twice, b13 143°. The m. p. of mixts. of the picrates of XXIX and XXX, and of the styphnates of XXIX and XXX show that XXIX and XXX are identical. Preparation of 1,2,8- trimethylnaphthalene (XL) (with J. Hartnagel and W. Hausschild): o-MeC6H4COCl (XLI) → o-MeC6H4COMe (XLII) → (+II) o-MeC6H4CMe(OH)CHMeCO2Et (XLIII) → Et (o-methyl)- α,α-dimethylcinnamate (XLIV) → 2-methyl-3-(o-tolyl)-1-butanol (XLV) → 1-bromo-2-methyl-3-(o- tolyl)butane (XLVI) → 1-cyano-2-methyl-3-(o-tolyl)butane (XLVII) → β-methyl-γ-(o-tolyl)valeric acid, (XLVIII) → β-methyl-γ-(o-tolyl)valeryl chloride (XLIX) → 1,2,8-trimethyl-4-keto-1,2,3,4-tetrahydronaphthalene (L) → XL. XLI + MeZnI → XLII, b10 86-9°; yield 75%. A solution of 19 g. XLI and 30 g. II in a little Et2O is added dropwise to 14 g. I-activated Zn turnings in absolute Et2O. The



solution is warmed to start the reaction and kept boiling vigorously for 5 hrs. The reaction product is cooled, poured into ice and HCl, extracted with Et2O, washed, dried and distilled in vacuo. Some unchanged XLII comes over first, then a mixture of XLIII and XLIV, b11 122-42°, which is dissolved in C6H6 and kept in contact with PBr3 24 hrs., washed with ice H2O and NaOH, and finally heated 1 hr. with PhNEt2 to split off HBr. XLIV, b11 128-32° (40 g.), is dissolved in a little absolute EtOH and added to 150g.Na. The mixture is warmed on the oil bath to 110-5° and just enough absolute EtOH added to permit solution of the Na. After 4 hrs. the alcoholate is decomposed with a little H2O and heated 30 min. to saponification unchanged XLIV. The EtOH is removed with steam and the residue extracted with Et2O. The Et2O is washed and distilled off, leaving XLV, b15 141-4°. Acidification of the wash water gives 15 g. α-methyl-γ-(o-tolyl)butyric acid, b15 170-6°, m. (recrystd. from MePh) 111°. XLV (14.4 g.) and 100 g. 33% HBr-AcOH (5 mols.) are heated 24 hrs. in a bomb at 100°. The liquid, which is clear at first and finally seps. into 2 layers, is poured into H2O and extracted with Et2O. The extract is washed with H2O and Na2CO3, dried and distilled; yield 17.5 g. XLVI, b14 134-40°. XLVI (17.4 g.), EtOH (360 g.) and 15 g. KCN (3 mols.) in 60 g. H2O are heated 16 hrs. on the water bath. After removing most of the EtOH, XLVII is extracted with Et2O. The crude XLVII is saponified directly by heating with 40 g. KOH dissolved in a min. of H2O and 200 g. MeOH in the autoclave 10 hrs. at 150°. The solution is acidified and XLVIII extracted with Et2O; yield 10 g., b14 183-4°, b0.7 140.5-1°. Ten g. XLVIII and 15 g. SOCl2 are heated on the water bath. At the end of the reaction the excess SOCl2 is removed and the XLIX distilled; b15 149°, yield 10.7 g. Fifteen g. powdered AlCl3 covered with freshly distilled CS2 is slowly mixed with 10.7 g. XLIX in the same weight CS2 and heated on the water bath until the evolution of HCl ceases. L is recovered as in the foregoing prepns.; yield 8.3 g., b19 162-6°. The semicarbazone of L m. 225-7° (decomposition), recrystd. from EtOH. L (3.25 g.) is reduced with Na and absolute EtOH to 2.8 g. of an oil, b16 140-56°. This is heated with 10 g. dry Se 56 hrs. at 300-30°, yield 1.9 g. XL, b16 150° (approx.). Preparation of 1,3,7-trimethylnaphthalene (LXI) (with P. Pieth and R. Thomann): p-tolualdehyde + II in the presence of Zn in C6H6 → Et β-(p-tolyl)-β-hydroxy-α-methylpropionate (LXII), b11 159-60°, b15 168°; 90% yield. LXII → Et p-methyl-α-methylcinnamate (LXIII) → 3-(p-tolyl)-2- methylpropanol (b12 129°) → γ-(p-tolyl)-β- methylpropyl bromide (b12 125°) → γ-(p-tolyl)-β-methylbutyronitrile → γ-(p-tolyl)-β-methylbutyric acid (b8.5 167-71°) → γ-(p-tolyl)-β-methylbutyryl chloride (LXIV), b9 131-2° → 3,7-dimethyl-1-keto-1,2,3,4- tetrahydronaphthalene (LXV) → 1,3,7-trimethyl-3,4-dihydronaphthalene (LXVI) → LXI, b9 131-3°, d421 0.9801, nD15.5 1.5972. After bromination of LXII with PBr3, HBr is split off with PhNMe2 to give LXIII, b12 149°. LXIV → LXV, b10 139°, m. 47°, when treated with AlCl3 in CS2; yield 90%. The semicarbazone of LXV, recrystd. (platelets) from MeOH, m. 204° (decomposition). The reaction product of LXV + MeMgI distilled over I and then distilled over Na → LXVI, b10 115-7°. LXVI heated 33 hrs. with its own weight of Se at 300-30° → LXI, which is purified by distillation over Na. Preparation of 1,4,5-trimethylnaphthalene (LXVII) (with E. Hefti and A. Ramon Altuna): p-xylyl Me ketone (Ber. 18, 1856(1895)) + II → Et 2,5-dimethyl-β-methylcinnamate, b12 148-50° → 3-(2,5-dimethylphenyl)-1-butanol, b12 141° → 1-bromo-3-(2,5-dimethylphenyl)butane, b12 134-5° → γ-(2,5-dimethylphenyl)valeronitrile → γ-(2,5- dimethylphenyl)valeric acid, b12 170°, m. 113.5° → γ-(2,5-dimethylphenyl)valeryl chloride, b12 144-5° → 1,4,5-trimethyl-8-keto-5,6,7,8-tetrahydronaphthalene, b12 138°, which is reduced with Na in absolute EtOH to 1,4,5-trimethyl-8-hydroxy-5,6,7,8-tetrahydronaphthalene, b12 128° → LXVII, b12 145°, m. 63° (recrystd. from MeOH). The procedures are the same as those for LXI. Preparation of 1,4,6-trimethylnaphthalene (LXVIII) (with W. H. Addink): p-MeC6H4COMe + II → Et p-

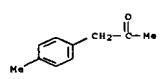


methyl-β-methylcinnamate, b15 158-60° → 3-(p-tolyl)-1-butanol, b15 150° → 1-bromo-3-(p-tolyl)butane, b20 140° → γ-(p-tolyl)valeronitrile → γ-(p-tolyl)valeric acid, b0.5 155° → γ-(p-tolyl)valeryl chloride, b12 145-7° → 1,6-dimethyl-4-keto-1,2,3,4-tetrahydronaphthalene, b15, 157-60° → 1,4,6-trimethyl-1,2-dihydronaphthalene, b13 135-8° → LXVIII, b15 140-2°. Preparation of 2,3,5-trimethylnaphthalene (LXIX) (with A. Weisz): Equal parts of o-MeC6H4CH2COCl and MePh are allowed to drop into MeZnI in ice-cooled Et2O. At the end of the reaction ice water is added, o-tolylacetone (LXX) recovered and distilled, b23 122°; yield 60%. LXX + II with Zn in C6H6 → a mixture, b14 130-70°, of unsatd. and HO acids which is treated with PBr3 and PhNMe2 to give Et α,β-dimethyl-γ- (o-tolyl)crotonate, o-MeC6H4CH3CMe:CMeCO2Et, b14 130-45°, which is reduced (Pt catalyst) at 80° to Et α,β-dimethyl-γ- (o-tolyl)butyrate (LXXI), b12 143-8°. LXXI is saponified to the acid (LXXII), b10 177°, with KOH-EtOH. LXXII → α,β-dimethyl-γ-(o-tolyl)butyryl chloride, b11 144-6° → 2,3,5-trimethyl-1-keto-1,2,3,4- tetrahydronaphthalene, b11 148°, which is reduced with Na in EtOH to 2,3,5-trimethyl-1-hydroxy-1,2,3,4-tetrahydronaphthalene (LXXIII), b12 142°, approx. LXXIII is dehydrogenated by heating with Se to give LXIX which, purified by distillation over Na, N2 138°. Preparation of 2,3,6-trimethylnaphthalene (LXXIV) (with A. H. Rierink): NaOEt (34 g.) is added to a mixture of 90 g. II and 60 g. p-tolualdehyde during 3 hrs. The mixture (cooled with ice-NaCl during the addition and overnight) is allowed to stand 2 hrs. at room temperature and finally heated 6 hrs. on the water bath. The product is decomposed with ice water, acidified with dilute AcOH and extracted with Et2O. The Et2O solution is washed and dried, the Et2O removed and Et α-methyl-β-(p-tolyl)-α,β-oxidopropionate (LXXV) distilled over, b12 148-52°; yield 62.5 g. LXXV is saponified by heating 3 hrs. with 7 g. Na in 150 cc. EtOH. The product is diluted with H2O and the EtOH removed with steam. After acidification α-methyl-β-(p- tolyl)-α,β-oxidopropionic acid (LXXVI) is taken up in Et2O, washed and dried. The Et2O is removed and LXXVI is decarboxylated by heating 24 hrs. at 180° to give p-tolylacetone (LXXVII), b12 109-10°; yield 41.8 g. LXXVII, II and Zn turnings in C6H6 → a mixture of HO and unsatd. acids, b12 150-70°, which is completely dehydrated by treatment with PBr3 and PhNMe2 to give Et α,β-dimethyl-γ-(p-tolyl)crotonate (LXXVIII), b13 158-63°. LXXVIII in AcOEt is reduced catalytically (Pt) to Et α,β-dimethyl-γ-(p-tolyl)butyrate, b7 148-51°, which is saponified to the acid (LXXIX), b0.6 148-50°. LXXIX → α,β-dimethyl-γ-(p-tolyl)butyryl chloride, b12 140° → 2,3,6-trimethyl-4-keto-1,2,3,4-tetrahydronaphthalene, b12 152-4° → 2,3,6-trimethyl-4-hydroxy-1,2,3,4- tetrahydronaphthalene → LXXIV, b14 146-8°. An incompleted preparation of LXXIV (with R. Delbes): LXIII in AcOEt is reduced (Pt) to Et α-methyl-β-(p-tolyl)propionate, b10 130-32°, which is sapond to the acid, b9 168-9° → α-methyl-β-(p- tolyl)propionyl chloride (LXXX). LXXX heated with MeZnI in Et2O → 1-(p-tolyl)-2-methylbutan-3-one, b11 124-7°, which is reduced with Na in abs.EtOH to 1,2-dimethyl-3-(p-tolyl)-1-propanol (LXXXI), b10 135-7°. LXXXI is heated at 100° with 30% HBr-AcOH. Upon distillation of the reaction product a poor yield (10%) of the expected bromide was obtained and it was concluded that LXXXI had been dehydrated. The synthesis was discontinued at this point.

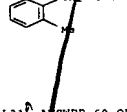
IT 2096-86-8P, 2-Propanone, 1-p-tolyl- 51052-00-7P, 2-Propanone, 1-o-tolyl-
RL: PREP (Preparation)
(preparation of)

RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)





RN 51052-00-7 CAPLUS
CN 2-Propanone, 1-(2-methylphenyl)- (CA INDEX NAME)



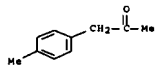
L31 ANSWER 60 OF 60 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1907:12321 CAPLUS Full-text
DN 1907:12321
OREF 1:3005e-i,3006a-i,3007a-b
TI Benzene Hydrocarbons With a Pseudo-Allyl Side Chain: Methovinyl Benzene and its Homologues. Study of Certain Molecular Migrations
AU Tiffeneau, M.
SO Ann. chim. phys., [8] (1907), 10, 145-98
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB The benzene hydrocarbons with a pseudo-allyl side chain may be made in general by the dehydration of the corresponding carbinol. They show the characteristic reactions of unsaturated hydrocarbons, giving dihalides and halodihydrins. The iodohydrins undergo a curious transformation when their ethereal solutions are treated with an excess of aqueous AgNO3, in that a ketone is formed; thus the iodohydrin of methovinylbenzene, C6H5CH3C(OH)CH2I, gives phenyl acetone, C6H5CH2COCH3, according to the equation C6H5CCH3(OH)CH2I=HI+C6H5CH2COCH3. With aqueous KOH the chlor- and iodohydrins give oxides; thus C6H5CCH3OHCH2I=C6H5CCH3CH2HI. Methovinylbenzene was obtained most satisfactorily by the dehydration of dimethylphenylcarbinol. The latter compound may best be made by the action of methylmagnesium iodide on methylbenzoate (Grignard, Ann. university Lyon, nouv. serie, 8, 73, (1901)), or by the action of acetone on phenylmagnesium bromide (Tissier and Grignard, Compt. rend., 132, 1182). The dimethylphenylcarbinol is purified by dissolving it in its volume of petroleum ether, cooling the solution and shaking continually until the carbinol separates in crystalline form. The dehydration of the carbinol to form the methovinyl benzene may be accomplished in a variety of ways: by slow distillation; by heat in the presence of a catalyzer, viz., Al2O3 or reduced Cu; by anhydrous oxalic acid. Methovinylbenzene may also be obtained by decomposing the product of the reaction of methylmagnesium iodide on acetophenone, or better, on ethyl or methyl benzoate. Alkalies decompose dimethylphenylchlormethane with the formation of methovinylbenzene.* Methovinylbenzene b. 161-162°. (See also Grignard, Ann. University Lyon, Nouv. serie, 100 (1901) ; Klages, Ber., 35, 2640 and 3507; Matsubara and Perkin, Jr., J. Chemical Society, 87, 668). By the action of H2SO4 on

methovinylbenzene a dimeride (See Grignard, Ann. University Lyon, 102, (1901), m. 51-52°, b14-15 163-164° is formed, or when a slight excess of methyliodide (only 1/2 mol. CH2MgI) is used a polymerideis also obtained, b10 175°, D0=1.012. (See Klages, Ber., 35, 2640). Methovinylbenzene is reduced to cumene by Na and absolute alcohol (Tiffeneau, Compt. rend., 134, 845), which furnishes a general method for the preparation of aromatic compounds having an isopropyl side chain. By passing it over reduced Ni, either cumene or hexahydrocumene is obtained, according to the activity of the Ni and length of time occupied in the process. Oxidation by air or KMnO4 gives acetophenone. α-Methylstyrolene dichloride, C6H5CClCH2.CH2Cl, is formed by action of Cl on methovinylbenzene, b15 119-121°, d0 1.2172. By heating with alcoholic KOH it gives β chloro-α-methylstyrolene, C6H5CCH3=CHCl, b. 210-215°, b14 102-106°. α-Methylstyrolene dibromide, C6H5CBrCH3CH2Br (Grignard, Matsubara and Perkin, Jr.), was made from methovinylbenzene and Br in ether, petroleum ether or CS2, b2 115-125°. ω-Bromoethylstyrolene, C4H5.C(CH3)=CHBr, is formed by the action of alcoholic KOH on the dibromide of methovinylbenzene or by Na2CO3 on methylcinnamic acid; b2 105-106°, b. 225-228° without decomposition, d0 1.366. Oxidation with KMnO4 in the cold gave acetophenone, which was characterized by its semicarbazone. This shows that the formula is C6H5CCH3=CHBr, rather than C6H5.CCH2Br=CH2, since the latter would give bromoacetophenone. Heated with KOH it gives phenylallylene. C6H5.C.tplbond.C.C6H5. With phenyl Mg bromide it gives methylstilbene. ω-Bromoethylstyrolene acts on metallic Mg in the presence of dry ether, and the product thus obtained on treatment with water gives a number of substances, viz., methovinylbenzene, phenylpropylene, phenylallylene and diphenyl-2,5-hexadiene-2,4, C6H5CH3C=CH.CH=CCH3C6H5. (See Tiffeneau, Bulletin society chim., [3] 26, 1186; Compt. rend., 135, 1346). By passing dry CO2 through the mixture obtained by action of Mg in dry ether, an addition product is obtained which on acidification gives two acids, one m. 97-98° and the other at 130°, which are probably the two stereoisomeric β-methylcinnamic acids. The acid which m. 97-98° has been obtained also by the dehydration and saponification of the product of the condensation of acetophenone with ethyl iodacetate in the presence of Zn or Mg (Tiffeneau, Compt. rend., 138, 985). Treated with HI it gives dihydromethylcinnamic acid and at the same time cumene is formed by the loss of CO2. Addition of hypochlorous acid gives a small quantity of methylphenylchlorlactic acid and methylchlorstyrolene. Chlorhydrin of methylphenylglycol, C5H2CH3COH.CH2Cl, b19 124-125°, d0 1,168. With dimethlamine it gives the dimethylamino derivative; (Fourneau, Compt. rend., 138, 736) with diethylamine, diethylaminophenyl-2-propanol-2, C6H5CH2COHCH2N(C2H5)2, b23 138-140°. The cinnamyl derivative m. 190-192°. Bromhydrin of methylphenylglycol, C6H5CH3COHCH2Br, b10 141°, d 1.413. Iodohydrin, b12 144-145°, d 1.541. It gives the same amino alcohol with methylamine as that given by the chlorhydrin, establishing its analogous constitution. These chlor- and iodohydrins on heating with aqueous KOH give the oxide of methovinylbenzene C6H5CCH3CH2, b16 84-85°, d0 1.043. This is easily isomerized into hydratropic aldehyde. The iodohydrin in ethereal solution when agitated with concentrate AgNO3 solution in excess, loses HI, and undergoes a curious transformation into phenylacetone. It was found that substitution in the benzene ring did not affect the nature of the transformation. o-Methovinyltoluene, CH3C4H4.C(Me)=CH2, b. 168-169°, was made by dehydrating dimethyl-o-tolyl carbinol, m. 41°, which can be obtained either by the action of acetone on the Mg compound of o-bromtoluene or methyl-Mg iodide on methyl o-toluate. Distillation with oxalic acid gives o-β-allyltoluene, b. 168-169°, d0 0.0076, which on oxidation with KMnO4 yields o-tolylmethylketone, b. 216°. The iodohydrin with AgNO3 gives by molecular transposition, o-tolylacetone, b. 227°; oxime, m. 75°, semicarbazone, m. 181°. m-Methovinyltoluene, b. 183-185°, d0 0.9115. The iodohydrin gives with AgNO3 m-toluyl acetone, b. 228-229°. Semicarbazide, m. 139°. p-Methovinyltoluene, b. 184-185°, d 0.9122, (Errara, Gazz. chim. ital., 31, 88 gives b. 198-200°) has odor of thyme. Dibromide does

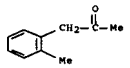


not crystallize at -15°. Heated with water and BaCo2, it gives the glycol, m. 32°. With H2SO4 it gives a dimeride, m. 40°. The iodohydrin is transformed into p-tolylacetone, b. 232-233°, giving oxime, m. 90°, and semicarbazone, m. 158°. Dimethylamine converts the iodohydrin into the corresponding p-tolylmethyldimethylaminoethylcarbinol, b. 253°-255°, d0 0.982.

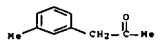
IT 2096-86-8, 2-Propanone, 1-p-tolyl- 51052-00-7, 2-Propanone, 1-o-tolyl-
(and derivs.)
RN 2096-86-8 CAPLUS
CN 2-Propanone, 1-(4-methylphenyl)- (CA INDEX NAME)



RN 51052-00-7 CAPLUS
CN 2-Propanone, 1-(2-methylphenyl)- (CA INDEX NAME)



IT 18826-61-4P, 2-Propanone, 1-m-tolyl-
RL: PREP (Preparation)
(preparation of)
RN 18826-61-4 CAPLUS
CN 2-Propanone, 1-(3-methylphenyl)- (CA INDEX NAME)



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